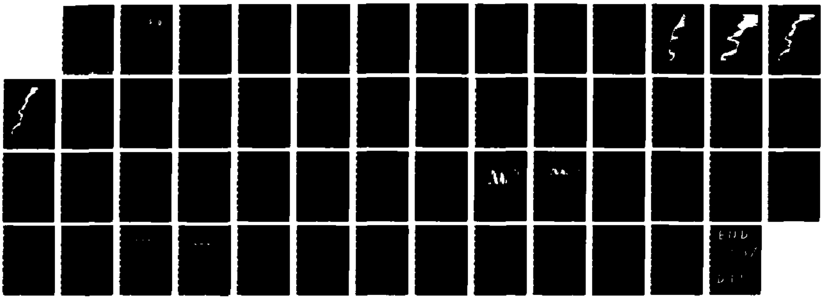
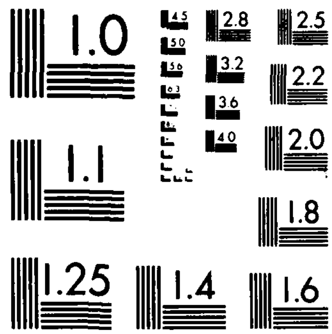
AD-A184 837 SPECTROSCOPIC AND RETRIEVAL STUDIES IN SUPPORT OF SCRIBE (STRATOSPHERIC C (U) ATMOSPHERIC AND ENVIRONMENTAL RESEARCH INC CAMBRIDGE MA 1/1

UNCLASSIFIED L D KAPLAN ET AL 08 MAR 87 P173F F/G 4/1 NL





MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

AFGL-TR-87-0084

Spectroscopic and Retrieval Studies in Support of SCRIBE

L. D. Kaplan
R. G. Isaacs
R. D. Worsham

Atmospheric and Environmental Research, Inc.
840 Memorial Drive
Cambridge, MA 02139

March 1987

Final Report
8 August 1986-8 February 1987

APPROVED FOR PUBLIC RELEASE; DISTRIBUTION UNLIMITED

AIR FORCE GEOPHYSICS LABORATORY
AIR FORCE SYSTEMS COMMAND
UNITED STATES AIR FORCE
HANSCOM AIR FORCE BASE, MASSACHUSETTS 01731

"This technical report has been reviewed and is approved for publication"

Michael Hoke

MICHAEL HOKE
Contract Manager 30 July 87

George A. Vanasse

GEORGE A. VANASSE, Chief
Infrared Physics Branch

FOR THE COMMANDER

Donald E. Bedo

DONALD E. BEDO, Acting Director
Optical Physics Division

This report has been reviewed by the ESD Public Affairs Office (PA) and is releasable to the National Technical Information Service (NTIS)

Qualified requestors may obtain additional copies from the Defense Technical Information Center. All others should apply to the National Technical Information Service.

If your address has changed, or if you wish to be removed from the mailing list, or if the addressee is no longer employed by your organization, please notify AFGL/DAA, Hanscom AFB, MA 01731. This will assist us in maintaining a current mailing list.

Do not return copies of this report unless contractual obligations or notices on a specific document requires that it be returned.

Unclassified
SECURITY CLASSIFICATION OF THIS PAGE

AD-A181 627

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION Unclassified	1b. RESTRICTIVE MARKINGS
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; Distribution unlimited
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S) P173F	5. MONITORING ORGANIZATION REPORT NUMBER(S) AFGL-TR-87-0084
6a. NAME OF PERFORMING ORGANIZATION Atmospheric and Environmental Research, Inc. 6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION Air Force Geophysics Laboratory
6c. ADDRESS (City, State, and ZIP Code) 840 Memorial Drive Cambridge, MA 02139	7b. ADDRESS (City, State, and ZIP Code) Hanscom AFB Massachusetts 01731
8a. NAME OF FUNDING/SPONSORING ORGANIZATION Air Force Geophysics Laboratory 8b. OFFICE SYMBOL (If applicable) AFGL/OPI	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER F19628-86-C-0172
8c. ADDRESS (City, State, and ZIP Code) Hanscom AFB, MA 01731	10. SOURCE OF FUNDING NUMBERS PROGRAM ELEMENT NO. 65502F PROJECT NO. 5502 TASK NO. 03 WORK UNIT ACCESSION NO. AE

11. TITLE (Include Security Classification)

Spectroscopic and Retrieval Studies in Support of SCRIBE

12. PERSONAL AUTHOR(S)
L. D. Kaplan, R. G. Isaacs, R. D. Worsham

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Final	FROM 8/8/86 TO 2/8/87	8 March 87	52

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	Retrievals, Remote Sensing, Line Coupling

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

A FASCODE-based physical retrieval algorithm for atmospheric temperature sounding is developed in support of data analysis for the SCRIBE high resolution interferometer using a modified version of FASCODE capable of treating highly opaque regions such as the CO_2 Q-branch at 667 cm^{-1}, radiances are simulated for comparison to SCRIBE data and the effects of line mixing are evaluated.

(keywords) —

20. DISTRIBUTION/AVAILABILITY OF ABSTRACT ☐ UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT ☐ DTIC USERS	21. ABSTRACT SECURITY CLASSIFICATION Unclassified
22a. NAME OF RESPONSIBLE INDIVIDUAL Michael Hoke	22b. TELEPHONE (Include Area Code) 22c. OFFICE SYMBOL AFGL/OPI

DD FORM 1473, 84 MAR — 83 APR edition may be used until exhausted. All other editions are obsolete.

SECURITY CLASSIFICATION OF THIS PAGE

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF FIGURES
(cont.)

1. Introduction

1.1. Background

The multiplex and throughput advantages of Fourier spectroscopy have made it possible to obtain rapid measurements of local emission spectra. The high resolution emission spectra that are available and will be coming from the Stratospheric Cryogenic Interferometer Balloon Experiment (SCRIBE) (Murcray et al., 1984, 1985) promise to provide important atmospheric information unattainable from solar occultation absorption spectra or other means. Of special interest are the diurnal variation of ozone-related trace gases in the stratosphere and anomalous variation with height of spectra in band passes used for temperature and compositional sounding, such as CO_2 Q-branches subject to line mixing. The SCRIBE data will also provide useful information for establishing the background radiation levels with which Air Force electro-optical systems must contend.

We proposed to begin, during the first phase of interpretation of SCRIBE spectra, three complementary investigations, namely, the validation of the spectra, the retrieval of trace gas profiles, and the retrieval of temperature profiles. Contracts were awarded both to us and to OPtiMetrics, Inc. This is fortunate, since there is much to be done with the spectra, and our program is ambitious. Efficiency required, however, that redundancy and duplication of effort be minimized. Our AFGL monitors suggested that OPtiMetrics have the primary responsibility for calibration and validation, while we concentrate on retrievals, particularly of temperature. We were happy to accept this plan of action.

Prior to commencement of the contract research, Professor Aaron Goldman of the University of Denver sent us samples of observed and synthetic data. From an examination of observed and synthetic spectra near the 15μm CO_2 Q-branch, we noticed that there appeared to be evidence for a substantial line coupling effect. The sign of the discrepancy seemed to be compatible with the departure of laboratory measurements at room temperature from synthetic laboratory spectra calculated by Dr. Michael Hoke, of AFGL's Optical Physics Division, for the same temperature, with and without line coupling.

Since this region of the spectrum is so important for remote sensing, and since there were no observed or calculated line coupling data at temperatures lower than room temperature, it was agreed that line coupling studies using SCRIBE data would have high priority in this first phase of the research, together with retrieval development and, of course, the adaptation of FASCOD2 (Clough et al, 1986) for calculation of synthetic SCRIBE spectra, which is necessary to carry out the other two objectives.

1.2 Technical Objectives of Study

This research proposed investigation of the potential of the unique SCRIBE high resolution spectra to provide information on atmospheric temperature and trace gas concentrations and to verify and validate spectroscopic modeling approaches such as that for line coupling. It was hoped that eventually these retrieval and spectroscopic studies could be extended to observations of the diurnal variations of trace gases and comparison of SCRIBE retrieved concentrations to those obtained from state-of-the-art photochemical models.

The technical objectives for this first phase of the study were thus threefold, as follows: (1) development of a FASCOD2 routine for the forward problem of calculating simulated radiances received at the SCRIBE altitude and angle-of-view; (2) using this routine to develop a FASCOD2-based temperature retrieval for SCRIBE data, and (3) investigating the effect of line coupling near the 15 μm Q-branch on FASCOD2 simulated radiance spectra and verifying this behavior in the SCRIBE data.

1.3 Report Overview

Chapter 2 below contains a brief description of the SCRIBE data, how it was obtained, calibration and noise problems, and the data subset that was used in our study.

Chapter 3 describes the SCRIBE temperature retrieval studies, starting with the forward problem calculations and development of a FASCOD2-based retrieval scheme adapted for SCRIBE. Channel selection and sensitivity studies with these provisional channels are described, and the chapter is concluded with an examination and discussion of preliminary retrieval results.

Chapter 4 discusses the investigation of the effects of line coupling on SCRIBE spectra in the vicinity of 15μm, as uncovered by our investigation. The effects are striking and may have important implications for remote sensing.

Finally, Chapter 5 contains a summary, and recommendations for future research.

2. SCRIBE Data Set

The SCRIBE instrument is a cryogenic Michelson interferometer spectrometer carried aloft by balloon for the purpose of observing the atmospheric emission spectra. It was flown in 1983, 1984 and 1986, each time obtaining spectra from 600 to 1500 cm^{-1} with a spectral resolution, after apodization, of 0.06 to 0.07 cm^{-1}. Each succeeding flight resulted in spectra with higher signal-to-noise ratio and easier to calibrate, but the 1986 data were not reduced and calibrated in time for us to work with them. The data for the flight on July 5, 1984, which was launched from Roswell, New Mexico, was available, however, and OPtiMetrics, Inc., provided us with magnetic tapes containing four "corrected" spectra from float elevation 30.5 km, at zenith angles 180 degrees (nadir), 88.1, 93.2 and 93.7 degrees. These are shown in Figs. 1 to 4, respectively, with the spectral region from 600 to 1500 cm^{-1} compressed to fit each spectrum onto a single page. Much of the spectra are seen to be quite noisy, even after correction, especially at the high frequency end, and a very prominent spike appears at 755 cm^{-1} on the 88.1 degree spectra. These features are not uncommon; in fact, these are presumably among the best spectra.

An even more serious problem for interpreting the spectra is that of calibration. A blackbody source was flown, but it seems to have encountered drifts. An idea of the magnitude of the calibration uncertainty can be obtained by comparing the four spectra at the common feature at 668 cm^{-1}, corresponding to the peak of the 15 μm CO_2 Q-branch. Here the atmosphere is so opaque at all angles that the measured radiances should be the same, corresponding to a brightness temperature equal to the ambient temperature at float altitude, which was measured by the White Sands, New Mexico, radiosonde to be very close to 230K. It can be seen, say by laying transparencies of the spectra one on the other, that the quasi-horizontally-viewed radiances agree

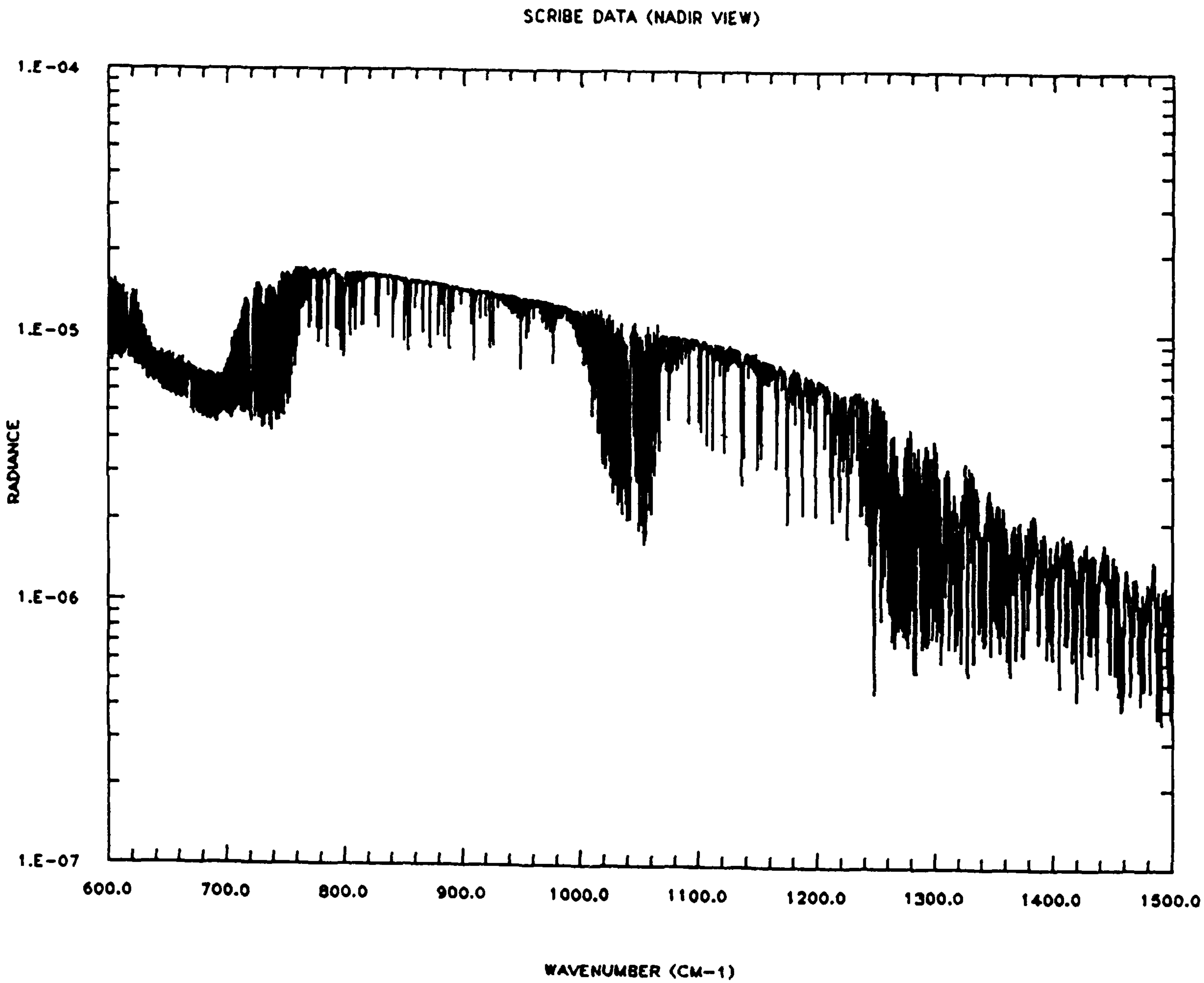


Figure 1 Corrected SCRIBE data, nadir view, 600-1500 cm^{-1}.

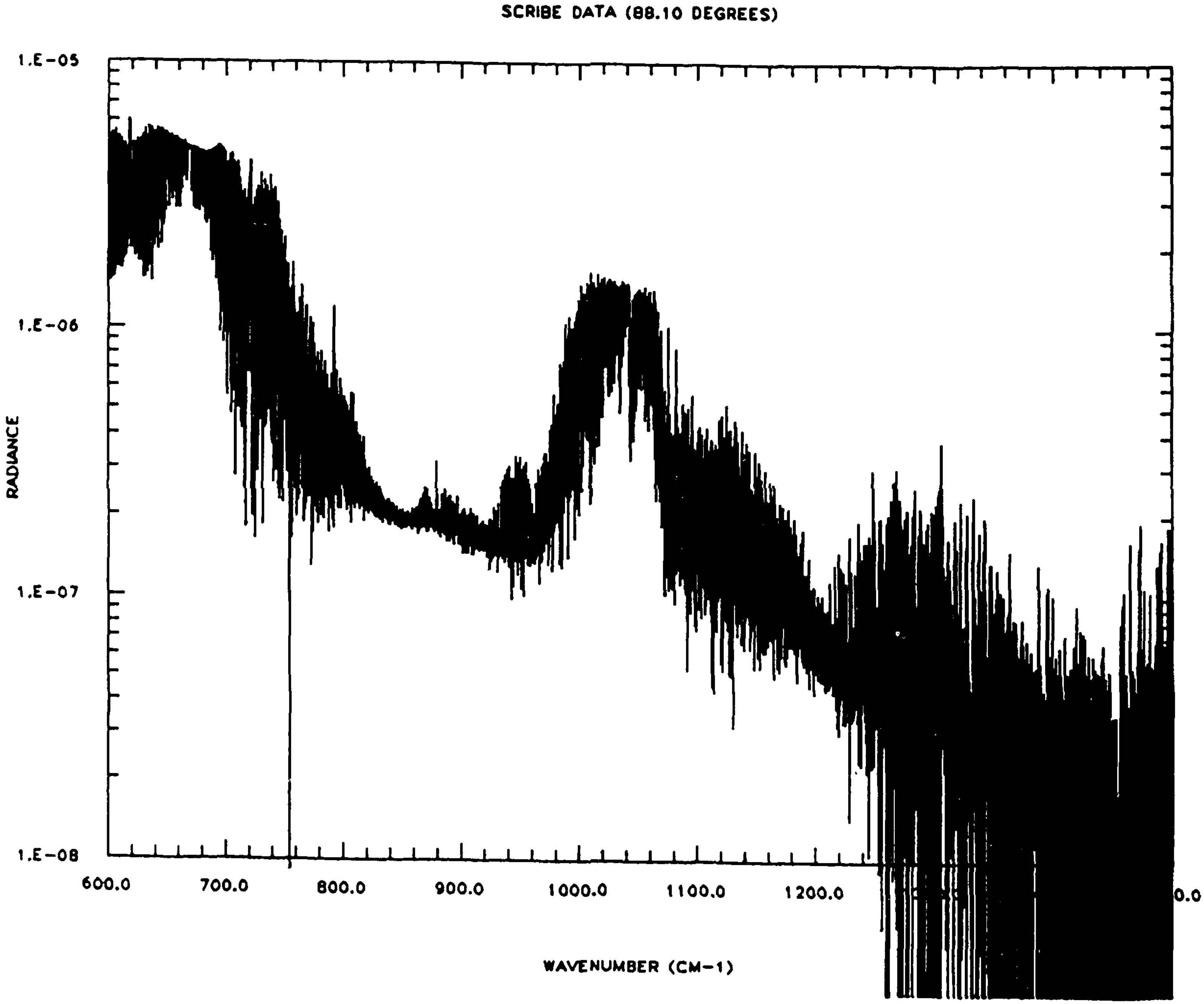


Figure 2 Corrected SCRIBE data, 88.1 deg, 600-1500 cm^{-1}.

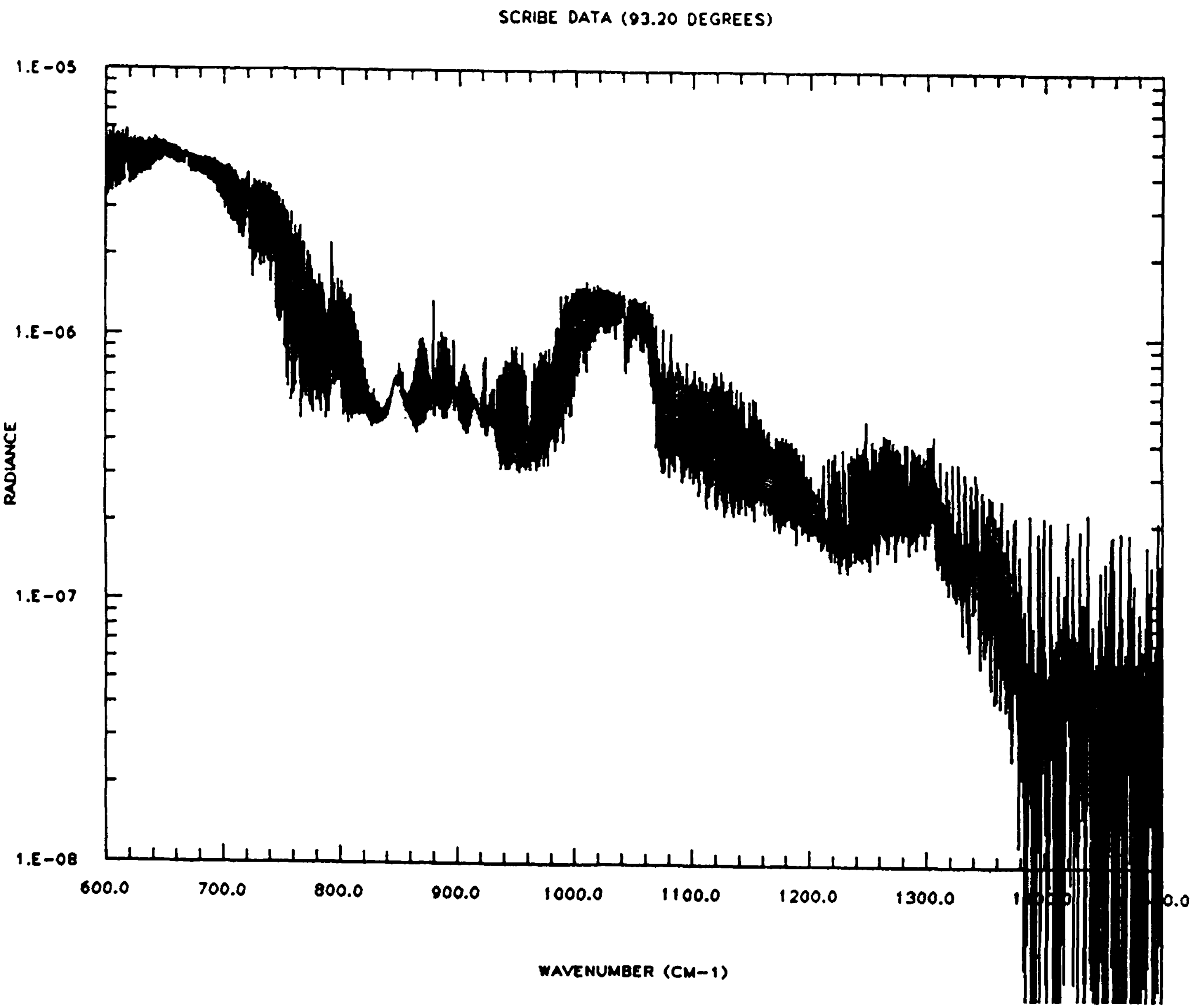


Figure 3 Corrected SCRIBE data, 93.2 deg, 600-1500 cm^{-1}.

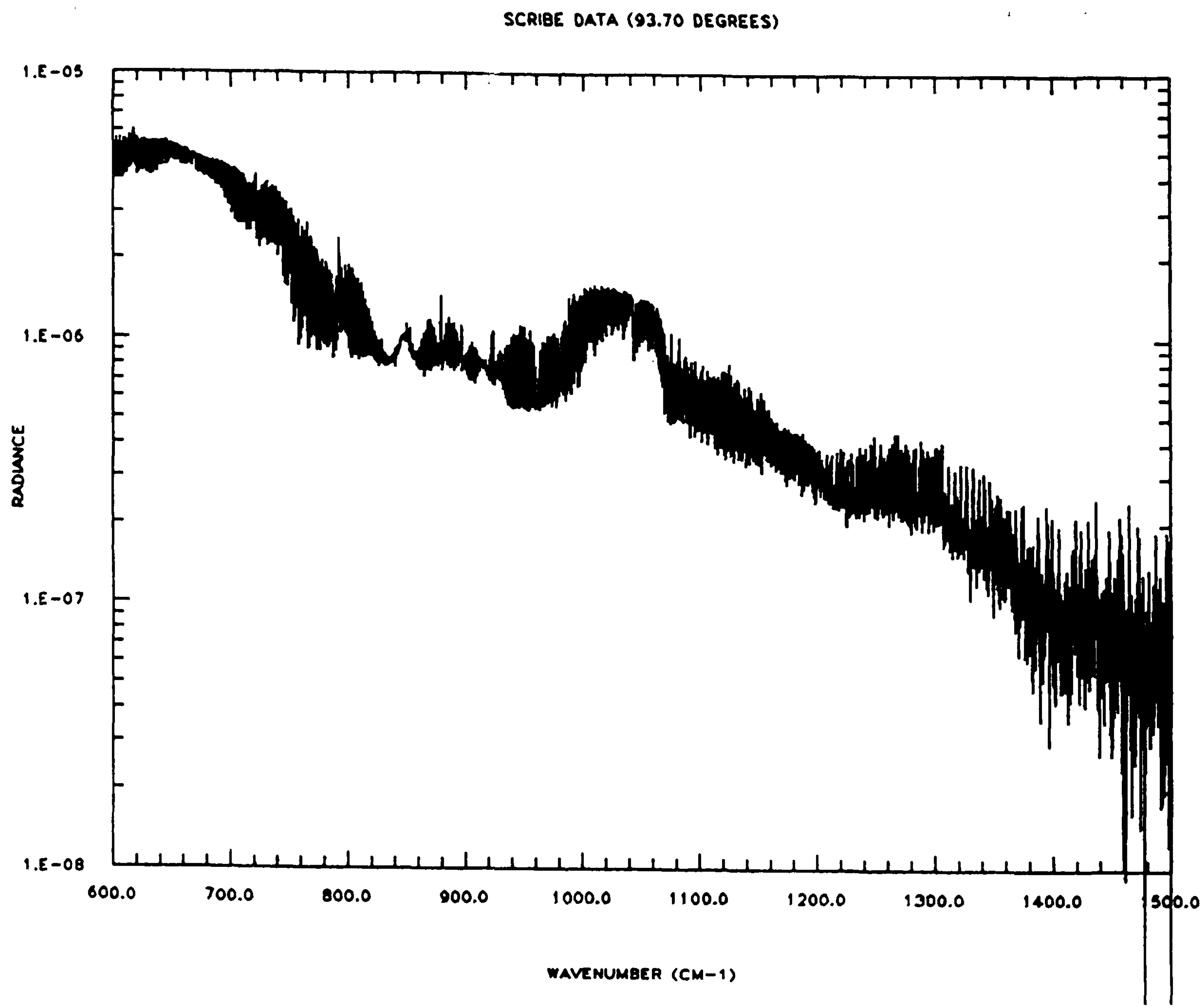


Figure 4 Corrected SCRIBE data, 93.7 deg, 600-1500 cm^{-1}.

with each other (the corresponding brightness temperatures are about 223K) but the radiance for nadir view is much higher, corresponding to a brightness temperature of about 250K. This can be seen in more detail in Figs. 23 and 30, below. Clearly great care should be taken with the calibration in interpreting the spectra, especially if the angular variation is used together with the spectral variation in retrievals.

In this study a small subset of the 1984 SCRIBE data was used. The spectral regions used were in the 15 μm CO_2 vibration-rotation band, more particularly between 600 to 670 cm^{-1}, since the retrieval studies and line coupling investigations fell within that spectral interval.

3. SCRIBE Temperature Retrieval Studies

3.1 Development of FASCOD2-Based Physical Retrieval for SCRIBE

Since no statistics were available relating radiances at SCRIBE level to atmospheric state variables, and since it would have required a prohibitive effort to acquire a set of synthetic statistics, a physical relaxation method was used in our temperature retrieval routine. This required forward computation of radiances. The availability of the AFGL line-by-line transmittance/radiance code FASCOD2 (Clough et al., 1986) was exploited to accomplish this step in formulating the physical retrieval approach. FASCOD2 enables the user to calculate high resolution, spectrally dependent transmittances and radiances by defining the relevant thermodynamic and compositional properties of the specific line-of-sight desired. Thus, appropriate data on the SCRIBE viewing geometry and first guesses for temperature and emitting gas concentrations could be used to initialize the retrieval procedure.

A variety of minor changes were required to tailor the application of the FASCOD2 model to our specific problem. FASCOD2's internal layering algorithm produced a set of layers for the vertical integration of radiance which was inappropriate for the observation geometry and spectral region of interest. Selected layers were too thick resulting in a suboptimal vertical quadrature. To better accommodate radiance calculations in the strongly absorbing spectral regions of interest, we apportioned the quadrature levels to be most closely spaced near the float level of 30.5 km, as follows for downward viewing: 0(1)28, 28.5, 29, 29.4, 29.7, 30, 30.2, 30.4, 30.5 km; i.e., 36 levels or 35 layers in all, which FASCOD2 easily accommodated.

We used Chahine's original form of the relaxation equation which, for the nth interation, relates the black-body radiance $B^{(n)}(p_j)$ for the levels p_j, corresponding to frequency ν_j, at which temperatures are retrieved, to the previous blackbody radiance $B^{(n-1)}(p_j)$ and to the measured and calculated radiances, R_j^* and $R_j^{(n-1)}$, respectively:

$$B^{(n)}(p_j) = B^{(n-1)}(P_j)R_j^*/R_j^{(n-1)} . \tag{1}$$

The process is continued as long as the calculated and observed radiances continue to converge or until their differences are approximately equal to the instrumental and computational noise.

The 15 μm band is the appropriate band within the SCRIBE spectral limits for atmospheric temperature sensing (Isaacs et al., 1986). Inherent in the full resolution SCRIBE data is considerable information pertaining to atmospheric temperature structure. Practical considerations, however, suggest the use of a small number of finite bandpass channels instead of the full resolution spectra. This approach makes the retrieval computationally tractable and improves signal-to-noise characteristics of the full resolution data. There is a trade-off, however, between bandpass weighting of the full resolution data and loss of atmospheric information inherent in the spectral variation of radiance. Therefore, the channel set selected has to be optimized with respect to these considerations.

Such a channel set for temperature sounding has been proposed in the engineering feasibility design stage of the Advanced Moisture and Temperature Sounder (AMTS) , a concept for future infrared satellite remote sensing of the atmosphere. We have adopted these preoptimized channels in this study of temperature retrieval from SCRIBE. The AMTS 15 μm atmospheric channels, are given in Table 1. from Chahine et al. (1984). These center frequencies were used for the SCRIBE retrieval and sensitivity studies. SCRIBE spectra and SCRIBE spectra simulated via FASCOD2 were spectrally integrated to the coarser AMTS channel resolution using triangular slit functions of 0.5 cm^{-1} full width at half height. Also given in Table 1 are the nominal peaks of weighting functions evaluated for these channels assuming a standard atmosphere and sensor viewing nadir from space.

Table 1. AMTS-based channel frequencies for SCRIBE temperature retrievals.

Channel Number	Frequency (cm-1)	Halfwidth (cm-1)	Weighting function Peak (mb)
1	606.95	0.5	850
2	623.20	0.5	700
3	627.80	0.5	400
4	634.30	0.5	270
5	646.60	0.5	180
6	654.35	0.5	90
7	665.55	0.5	70
8	666.85	0.5	30
9	668.15	0.5	3
10	669.45	0.5	20
11	875.00	0.5	900

The overall retrieval scheme developed for SCRIBE thus consists of the following steps:

(a) Full resolution SCRIBE spectra are degraded with a triangular slit function to give channel radiances at 0.5 cm-1 resolution for the sounding frequencies in Table 1; these are the resampled data

(b) First guess path temperature and constituent profiles are assumed based on a priori information or climatology and FASCOD2 is run (with the vertical layering modified for SCRIBE runs) to calculate a full resolution synthetic spectrum for the wavenumber domains of interest (those included in the channels of Table 1.

(c) The full resolution spectrum is degraded to give 0.5 cm-1 channel radiances.

(d) The synthetic radiances thus calculated are compared to the degraded SCRIBE data produced in step (a).

(e) The temperature profile is adjusted using Eqn. (1).

(f) The process is continued as long as the calculated and observed radiances continue to converge or until their differences are approximately equal to the instrumental and computational noise.

The success of the resulting retrieval depends on the levels of noise in the data, the quality of the first guess and the ability of the selected channel set to provide information on temperature variations along the observational path. Since FASCOD2 is used iteratively and interactively, a good first guess is important. The efficiency of the retrieval approach could be enhanced by developing a "rapid" algorithm to carry out the path transmittance calculations required for the forward problem. A rapid algorithm is essentially a band model specifically tuned for each of the desired synthetic sensor channels (e.g. Susskind et al., 1982). It is based on an ensemble of calculations performed with the exact line-by-line (LBL) code, i.e., FASCOD2. This task was not undertaken in Phase I due to the uncertainties in treatment of line coupling effects at this time.

3.2 Retrieval results

Two temperature retrievals were carried out. The first, to test the system, used the actual radiosonde sounding to compute synthetic "measured" radiances, and each channel was associated with the pressure at which the channel brightness temperature is equal to the corresponding temperature for a standard tropical atmosphere. An isothermal first guess was used, so that $B_j^{(n-1)} - R_j^{(n-1)}$ = constant in Eq. (1), and the first iteration should already give a reasonably good solution if the actual sounding is close to that for the standard tropical atmosphere,which it is in this case. Figure 5 shows that the solution has already converged to the correct sounding after only two iterations.

The second retrieval exercise was carried out using actual SCRIBE measured radiances. Data from the nadir scans illustrated in Figure 1 were selected for this test of the retrieval algorithm. To reconcile apparent calibration problems in the SCRIBE data, the actual spectra were scaled to give agreement with the blackbody radiance corresponding to ambient

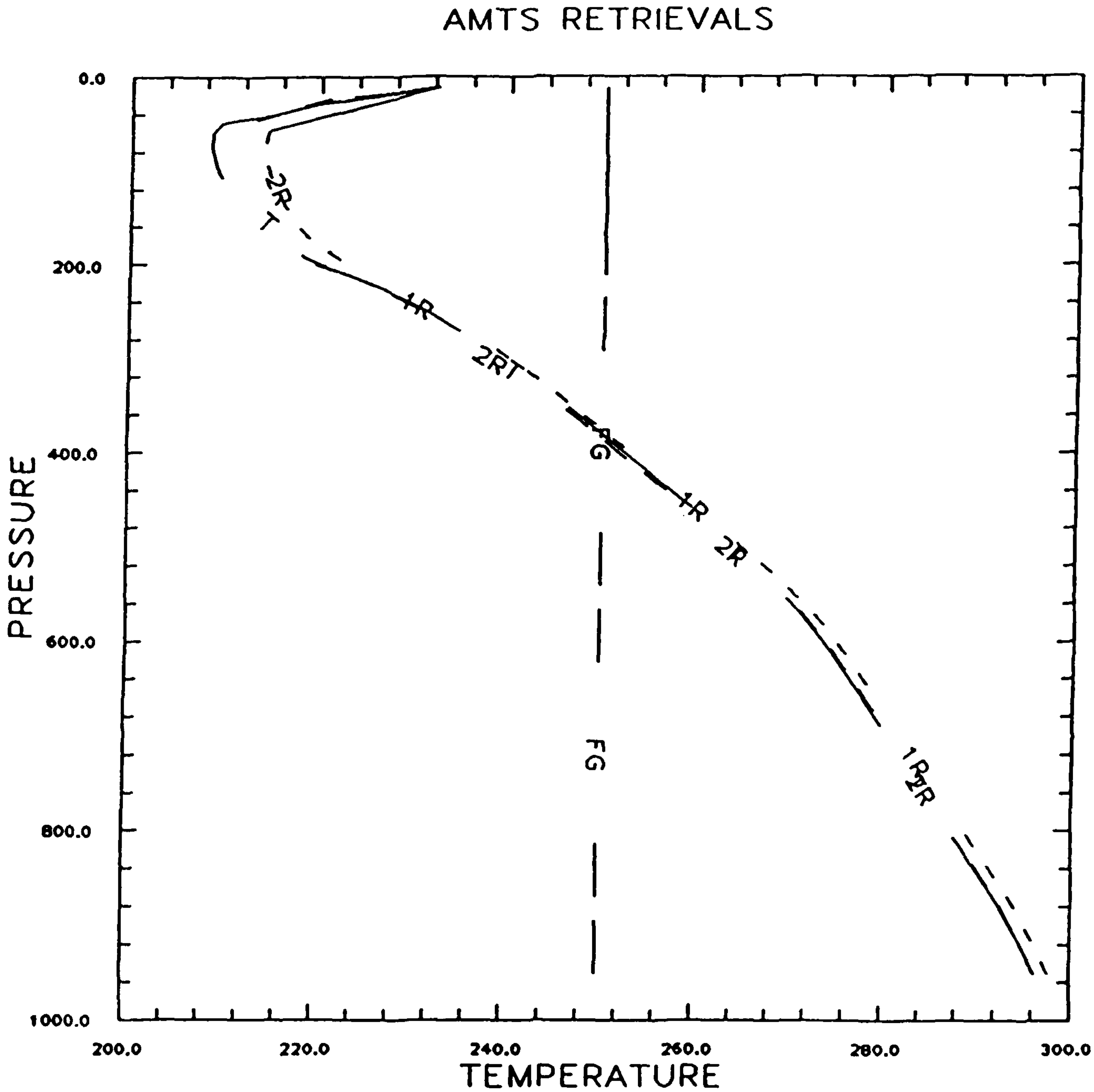


Figure 5 SCRIBE retrieval results, pressure-channel association from tropical atmosphere:

temperature at the peak of the 15 μm Q-branch. Ambient temperatures were obtained from the local radiosonde data obtained in support of the SCRIBE measurements. Although the sounding was obtained a few hours earlier, there should be little diurnal variation of temperature at the levels observed at the peak of the Q-branch, i.e. essentially float altitude.

In order to adjust the guess profile using the bandpass weighted data and simulations using Eq. (1), it is necessary to establish a one-to-one correspondence between channel residuals and required adjustments at a specified pressure level. The channels in this case were associated with the pressures at which their respective brightness temperatures were equal to the corresponding temperatures of a U.S. Standard Atmosphere. This atmospheric model was also employed as a first guess of the temperature profile to initiate the retrieval process. Results are shown in Figure 6. Using the radiosonde as a standard for comparison (the curve labelled "SCRIBE"), convergence is apparent in the general ranges between 10 and 30 mb, 200 and 400 mb, and in the vicinity of the surface. Figure 6 also shows that the results were quite poor in the lower stratosphere, probably because $B_j^{(n-1)}$ and $R_j^{(n-1)}$ in Eq. (1) are still equal, though no longer constant. This constrains any further relaxation of the lower stratosphere temperatures. One further suspects that there may be little information on temperature variation at these levels available from the set of selected channels.

It should be noted that considerable improvement can be obtained by extrapolating the lower stratospheric lapse rate downwards and the upper tropospheric lapse rate upward, and taking the intersection as the tropopause. But clearly better associations between channels and sounding levels are required. We have therefore devoted the rest of our remote sensing effort to sensitivity studies designed specifically for the SCRIBE data. These sensitivity studies and their results are described in the following section.

3.3 Sensitivity Studies

The sensitivity studies were carried out in the nadir viewing mode. For each set of sensitivity curves, synthetic upwelling SCRIBE radiances were calculated for each channel with the FASCOD2 forward program. The calculations were done for either a U.S. Standard or Standard Tropical Atmosphere, without perturbation and for each of a set of perturbed atmospheres obtained by increasing the temperature by 5C consecutively over a 1 km equivalent layer

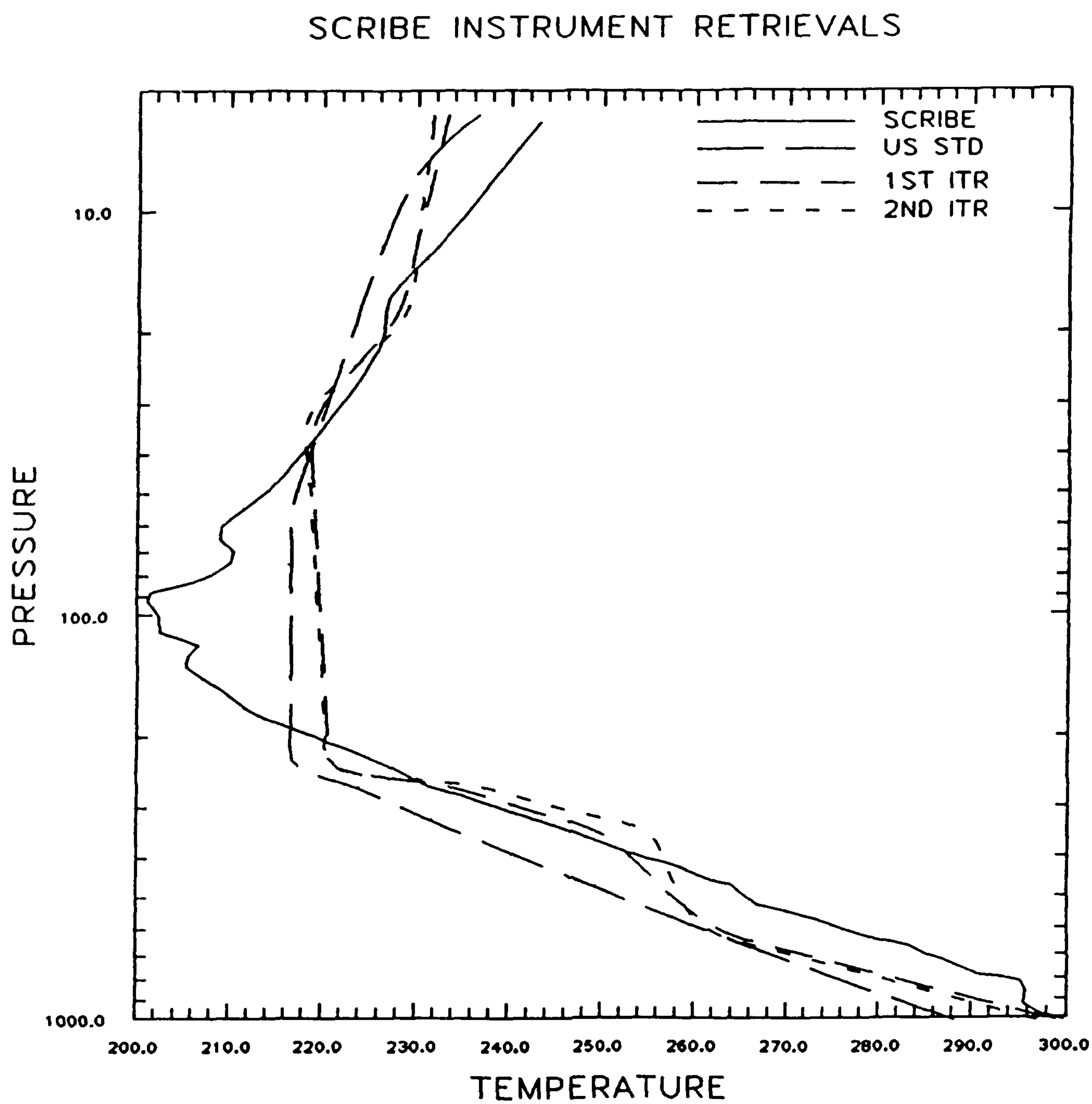


Figure 6 SCRIBE retrieval results, pressure-channel association from U.S. Standard Atmosphere:

thickness centered at the 16 levels 1(2)25(2.5)32.5 km, then subtracting the unperturbed from the perturbed brightness temperature. These brightness temperature differences are plotted as a linear function of height in Figures 7 to 16. They can be used to assign effective sounding heights to the various channels. The sets of sensitivity curves are remarkably similar to each other, regardless of model atmosphere used, which indicates that the same set of correspondences between channel and height can be used for all soundings. The differences are discussed below.

Figures 7 and 8 show the sensitivity curves for the U.S. Standard Atmosphere calculated from the line parameters on the 1982 HITRAN (Rothman et al., 1983) tape, for the troposphere and stratosphere, respectively. These can be compared with the sensitivity curves calculated using the latest (1985) HITRAN data shown in Figures 9 and 10. Line coupling was ignored in calculating these sets of sensitivity curves. The effect of updating the line parameter compilation is only evident for the 606.95 cm^{-1} channel, which is least dominated by the lines of the fundamental transition. The 606.95 cm^{-1} channel is redundant with the 623.2 cm^{-1} channel; otherwise the tropospheric channels are nicely spaced. The stratospheric channels, on the other hand, overlap markedly. Further examining Figures 7 and 8 it is notable that there is a minimum in sensitivity to temperature variations in the range between about 12 and 20 km; the single channel at 654 cm-1 provides some information. This corresponds to the pressure region between 60 and 200 mb where convergence problems were evident in the retrieval exercise described in the previous section. Clearly further work is required on channel optimization for the temperature profile retrieval problem.

Figures 11 and 12 were calculated like Figures 9 and 10, except that it was done for the Standard Tropical (M-1 in FASCOD2) rather than U.S. Standard Atmosphere. The tropical sensitivity curves are indistiguishable from the standard curves in the stratosphere, so it shows the same marked overlapping. Limb scanning would be much more appropriate for sounding the stratosphere. The tropical sensitivity curves for the troposphere are quite different from the standard curves, particularly in the region between tropical and standard tropopause, but the heights of the sensitivity curve maxima are almost unchanged. This suggests that a universal association of channel frequency ν with height z could be chosen somewhat as shown in Table 2 on page 22.

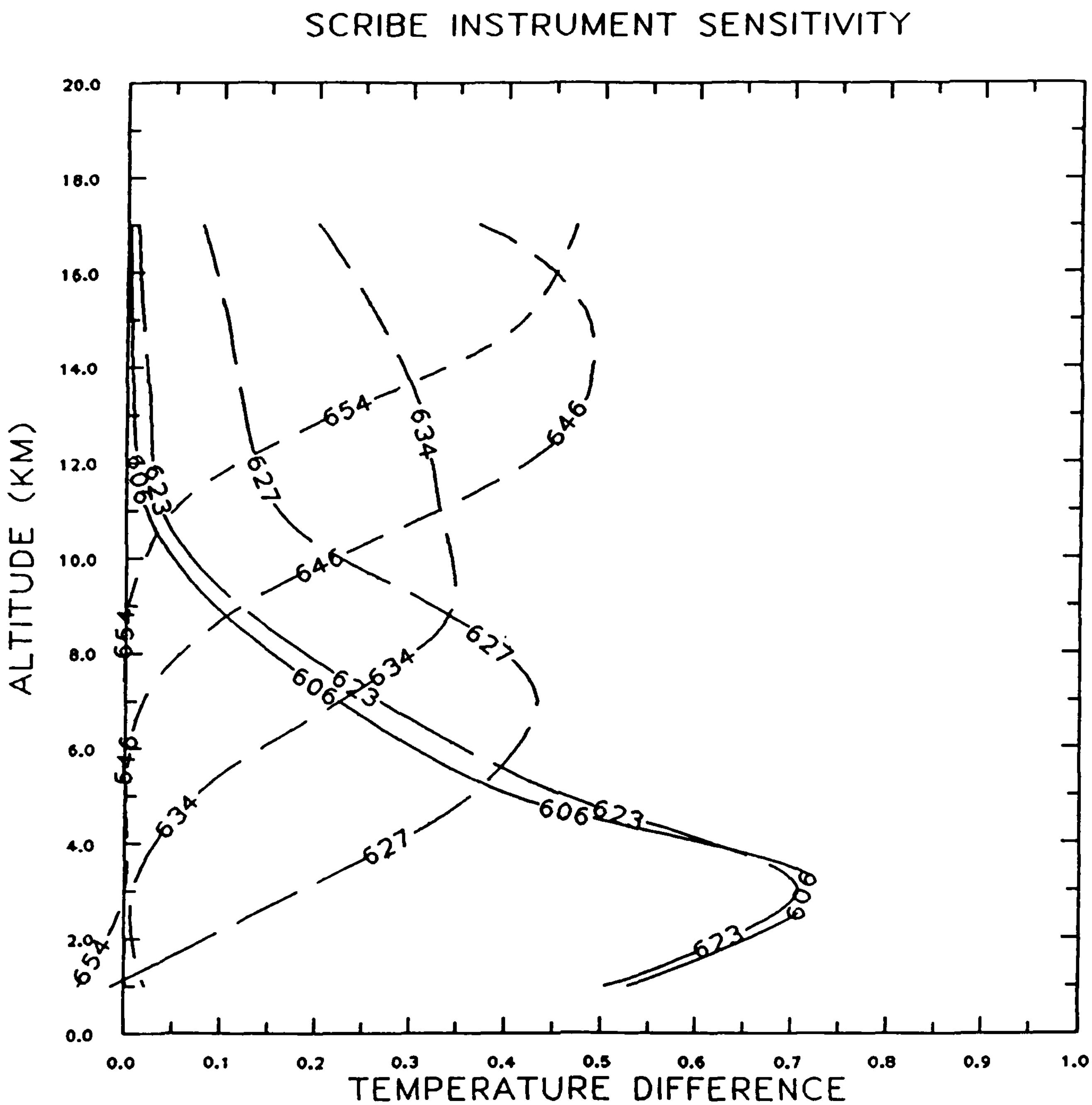


Figure 7 SCRIBE instrument sensitivity results: 606-654 cm^{-1} channels, old line data, US standard atmosphere, no line coupling.

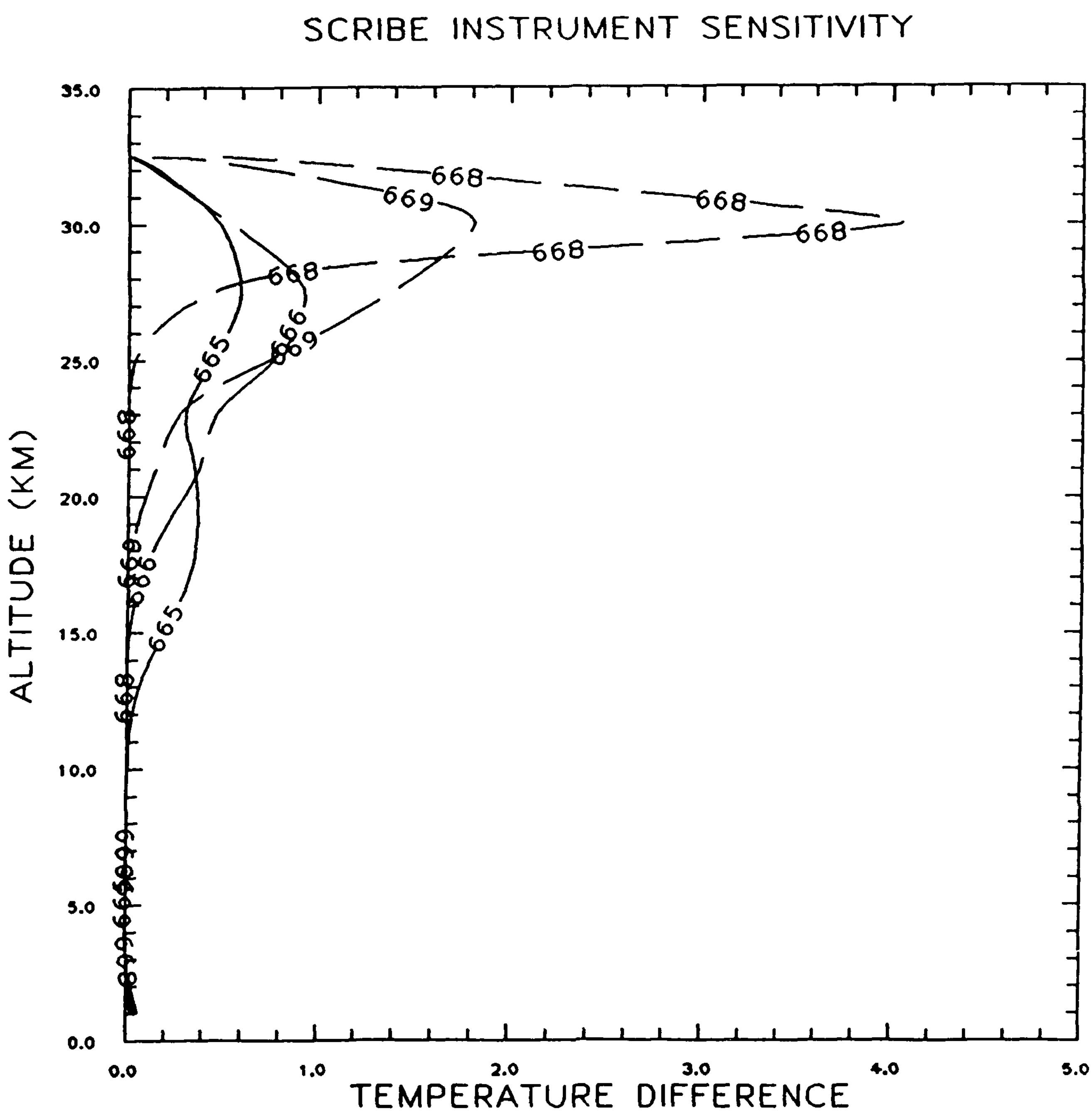


Figure 8 SCRIBE instrument sensitivity results: 665-669 cm^{-1} channels, old line data, US standard atmosphere, no line coupling.

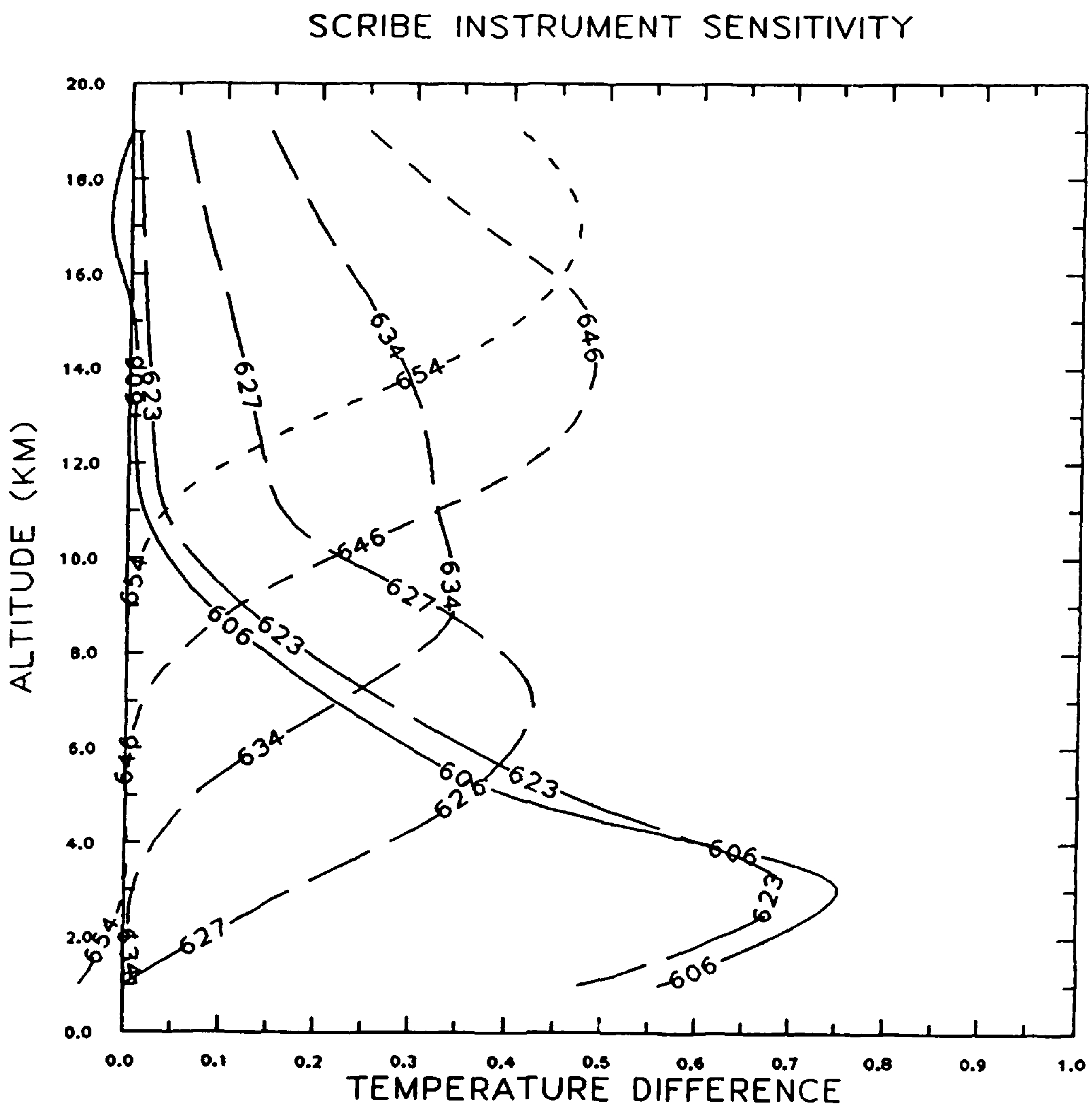


Figure 9 SCRIBE instrument sensitivity results: 606-654 cm^{-1} channels, new line data, US standard atmosphere, no line coupling.

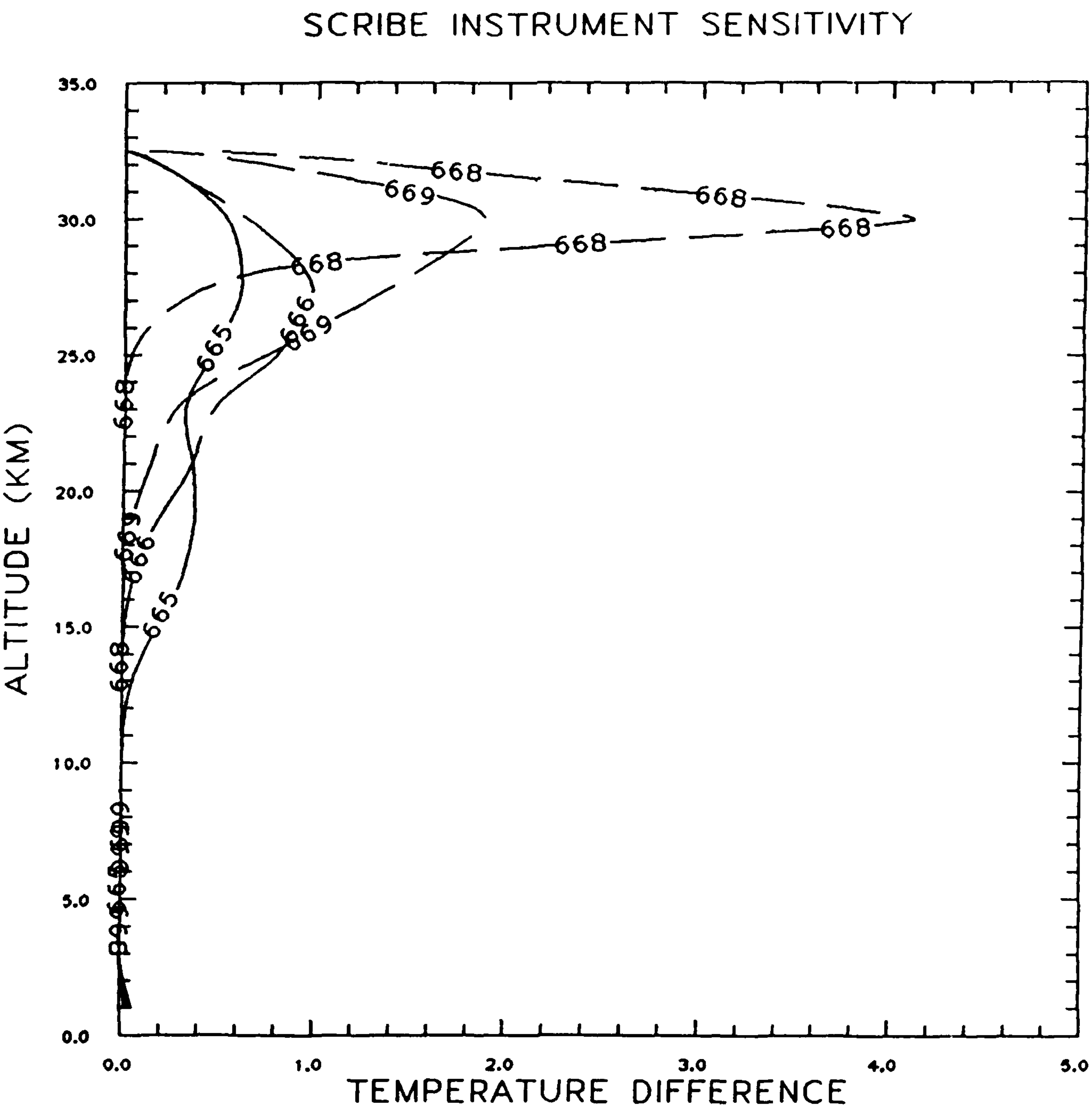


Figure 10 SCRIBE instrument sensitivity results: 665-669 cm^{-1} channels, new line data, US standard atmosphere, no line coupling.

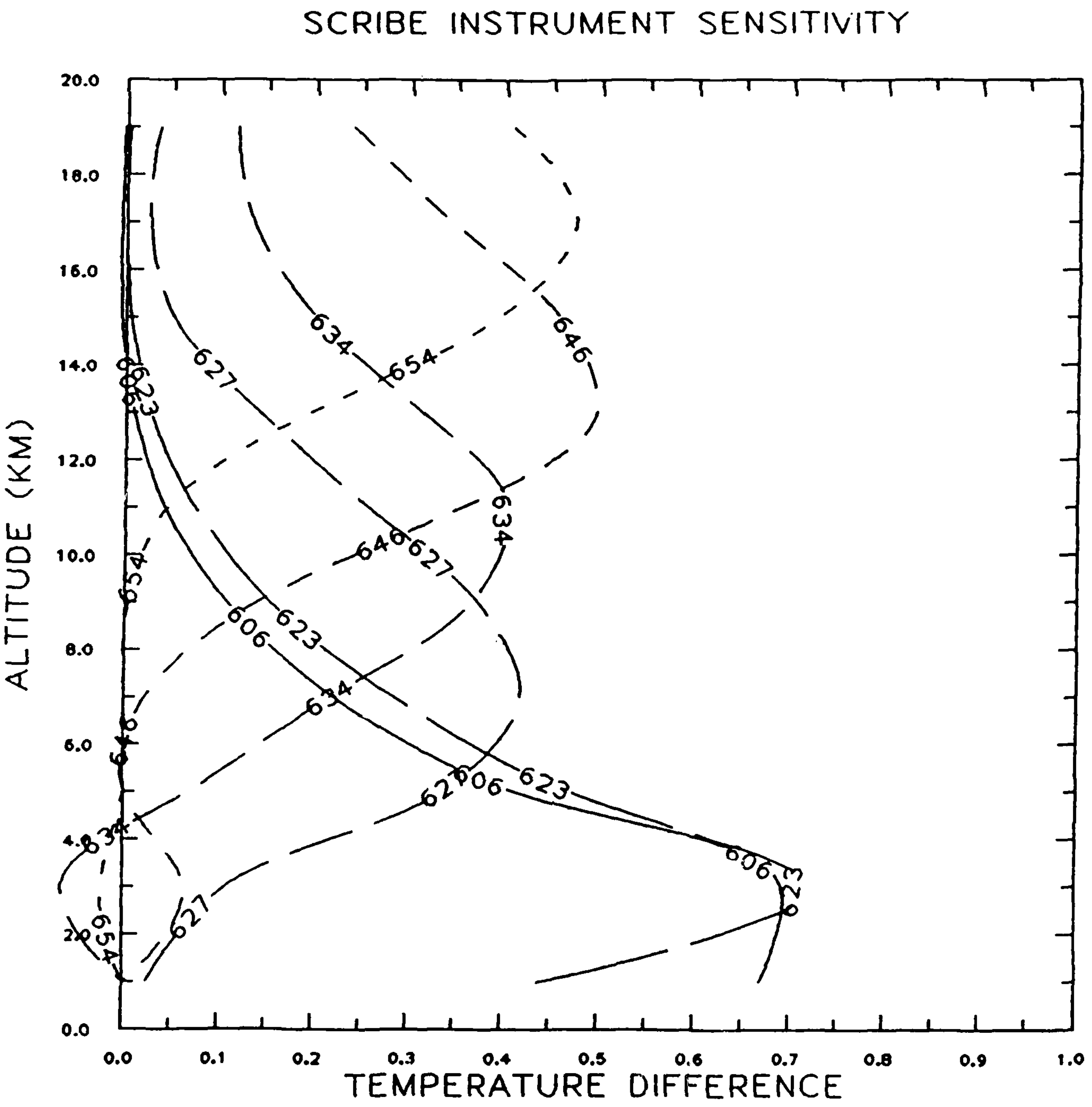


Figure 11 SCRIBE instrument sensitivity results: 606-654 cm^{-1} channels, new line data, tropical atmosphere, no line coupling.

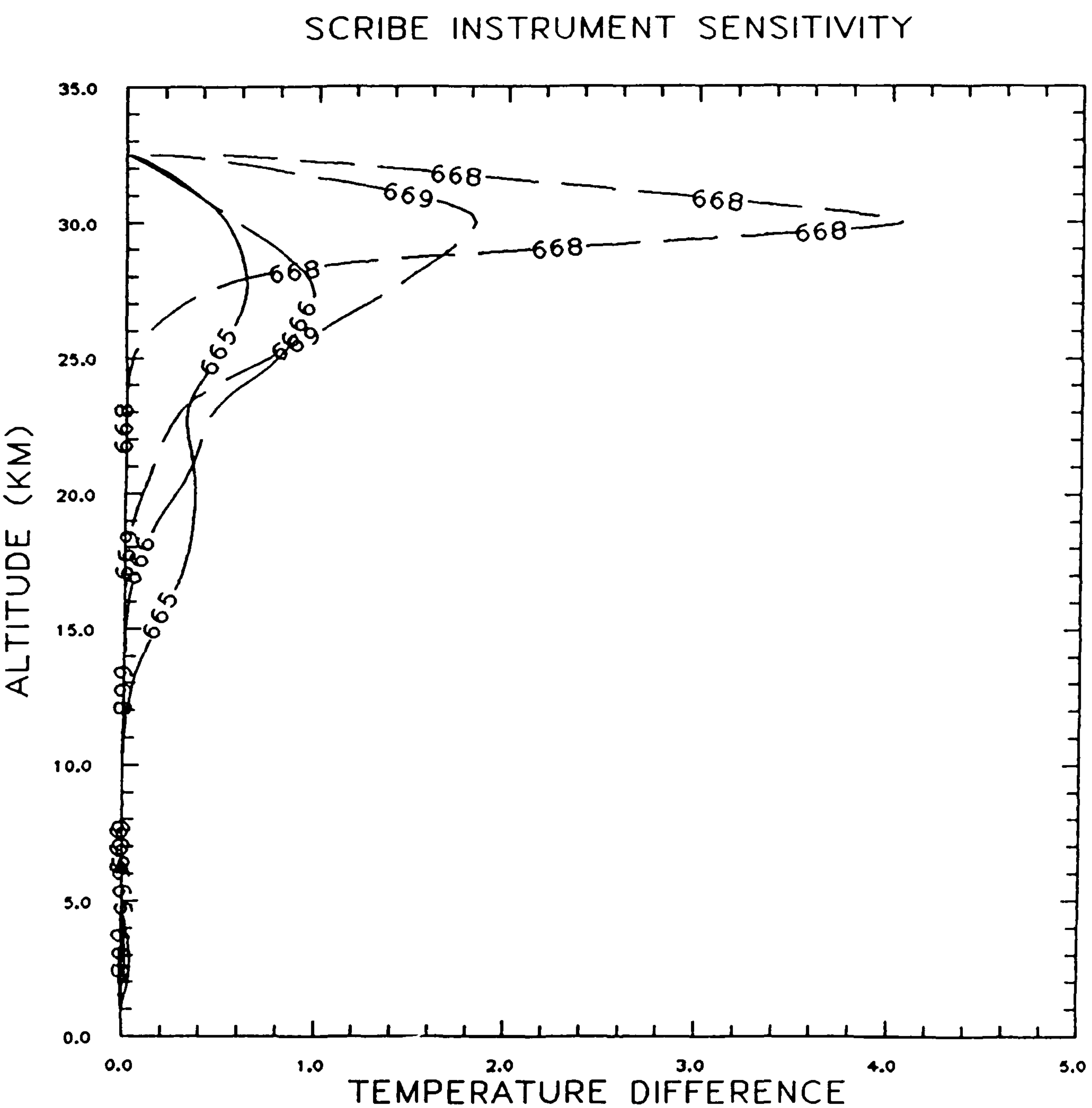


Figure 12 SCRIBE instrument sensitivity results: 665-669 cm^{-1} channels, new line data, tropical atmosphere, no line coupling.

Table 2. Association of channel frequency with altitude for retrieval application.

Channel	11	2	3	4	5	6	7	8	9	10
$\nu(cm^{-1})$	875	623.2	627.8	634.3	646.6	654.4	665.6	666.8	668.2	669.4
z(km)	1	3	7	11	14	17	(20)	27.5	29	30

Sensitivity curves were also calculated to investigate the effect of line coupling in the 15 μm Q-branch. These are presented in the following section.

4. Investigation of Line Coupling Phenomena with Scribe Data

4.1 Background

Line coupling is the distortion of the line shape as a result of the rapid rotational relaxation of closely spaced transitions, such as in Q-branches of perpendicular molecules such as CO_2, and perhaps even more so for molecules with larger moments of inertia and therefore more closely spaced lines. A discussion of this effect was given together with a bibliography, by M.L. Hoke and S.A. Clough of AFGL and W. Lafferty and B.W. Olson of NBS (National Bureau of Standards) at the 5-6 June 1986 Annual Review Conference on Atmospheric Transmission Models, in a paper entitled "Line Coupling in Carbon Dioxide". Drs. Hoke and Clough expanded the absorption coefficient to first order in pressure p, and compared calculated spectra of the CO_2 15 μm Q-branch with laboratory measurements. Their line shape for a line centered at ν_{if} was of the form

$$k(\nu,\nu_{if}) = \sum_{if} p\frac{S_{if}}{\pi}\,\frac{\alpha_{if} + y_{if}(\nu-\nu_{if})}{\alpha_{if}^{2}p^{2} + (\nu-\nu_{if})^{2}} . \tag{2}$$

This expression reduces to the Lorentz shape when the coupling coefficients Y are set to zero. The Y's used in the laboratory comparison were calculated for the laboratory temperature of 296 K, and are included in the latest HITRAN tape (Rothman, 1986). The introduction of line coupling almost eliminated a rather sizable discrepancy between observed spectra and spectra calculated with the use of a Lorentz line shape.

CO_2 line coupling near 15 μm has not been investigated at other than laboratory room temperature. The SCRIBE data, on the other hand, provide the opportunity to check calculations of the temperature dependence of line coupling, and its effect on atmospheric transmittance and radiances. This is especially important in the main Q-branch region, which is useful for retrieval of stratospheric temperatures.

Dr. Hoke kindly agreed to calculate Y values for the temperatures 210, 230, 260, 296, 330 , so that we could investigate the effect of temperature dependence variations on radiances and on the sensitivity curves.

4.2 Effect of Line Coupling on Sensitivity Curves

Sensitivity curves were calculated with line coupling included by using the line coupling option of FASCOD2. As currently formulated line coupling coefficients are stored in the space allocated in the line parameter compilation for pressure shifts. When non-zero values are encountered for this parameter the FASCOD2 algorithm calculates the appropriate correction to line shape using Eq. (2) above. To accomodate Hoke's temperature dependent line coupling coefficients, the line parameter compilation was edited to substitute the more recent values at, for example, 230K. Since only the Y's for the fundamental Q-branch were used, the major effects could be expected to be found for the channels sounding just below SCRIBE float altitude where the temperature 230K was representative.

It is important to note that this application of FASCOD2 uses the line coupling parameters for the chosen temperature for all layers, i.e. at all selected mean layer temperatures within the simulation. The calculation is therefore isothermal and does not fully exploit the capability to calculate temperature dependent line coupling coefficients. This can be accomplished, but only through an appropriate modification of the FASCOD2 algorithm to either accept temperature dependent line parameter data (i.e. line parameters for each layer) or by fitting a simple functional form to or scaling the line coupling coefficient temperature dependence so that it can be internally calculated as is currently done for line strength, for example.

The tropospheric and stratospheric results with line coupling, respectively, are shown in Figures 13 and 14 for the U.S. standard atmosphere and in Figures 15 and 16, respectively, for the standard tropical (M-1) atmosphere. When these sensitivity curves are compared with Figures 9 through 12 it is seen that potential effects of line coupling are evident on the sensitivity curves for the 666.8 cm^{-1} channel, but that the sensitivity curves for the other channels are relatively unaffected. To see why this is so for the stratospheric channels we must look at the spectrally detailed synthetic radiances shown in the figures to follow. The apparent insensitivity of the tropospheric channel radiances to line coupling is to be expected because we ignored all Q-branches except for the fundamental. The entire 15 μm band region is strewn with Q-branches separated from each other by accidental Fermi resonances. Thus the effect found for the 666.8 cm^{-1} channel may also appear in tropospheric or tropopause channels such as that at 646.6 cm^{-1}, which is very close to two Q-branches. This emphasizes the importance of line coupling to remote sensing and the necessity for extending the investigation of these sensitivities to other related Q-branches.

It should also be noted that even for the 666.8 cm^{-1} channel, the height of the peak of the sensitivity curve is unaffected by line coupling.

4.3 Comparison of SCRIBE Data to Synthetic Calculations

Detailed synthetic SCRIBE spectra were calculated using the modified FASCOD2 algorithm from 660 to 670 cm^{-1}. Line coupling effects were not included in the calculation due to the non isothermal nature of the emission path. Nadir brightness temperatures and radiances are shown in Figures 17 and 18, respectively. These can be compared to the corresponding observed SCRIBE nadir viewing spectra in Figures 19 and 20 (e.g Kelvins and radiance, respectively.) Here there is an obvious calibration problem, since the brightness temperature measured at the Q-branch maximum is close to 250K rather than the ambient temperature of 230K. When the measured radiances are shifted downward on a logarithmic radiance scale to peak at 230K at the maxima, and a window correction of five percent of ambient temperature is added, the resulting spectrum is reasonably similar to that for the synthetic spectra. This assumes that the synthetic spectra are first degraded in resolution to that of the SCRIBE instrument.

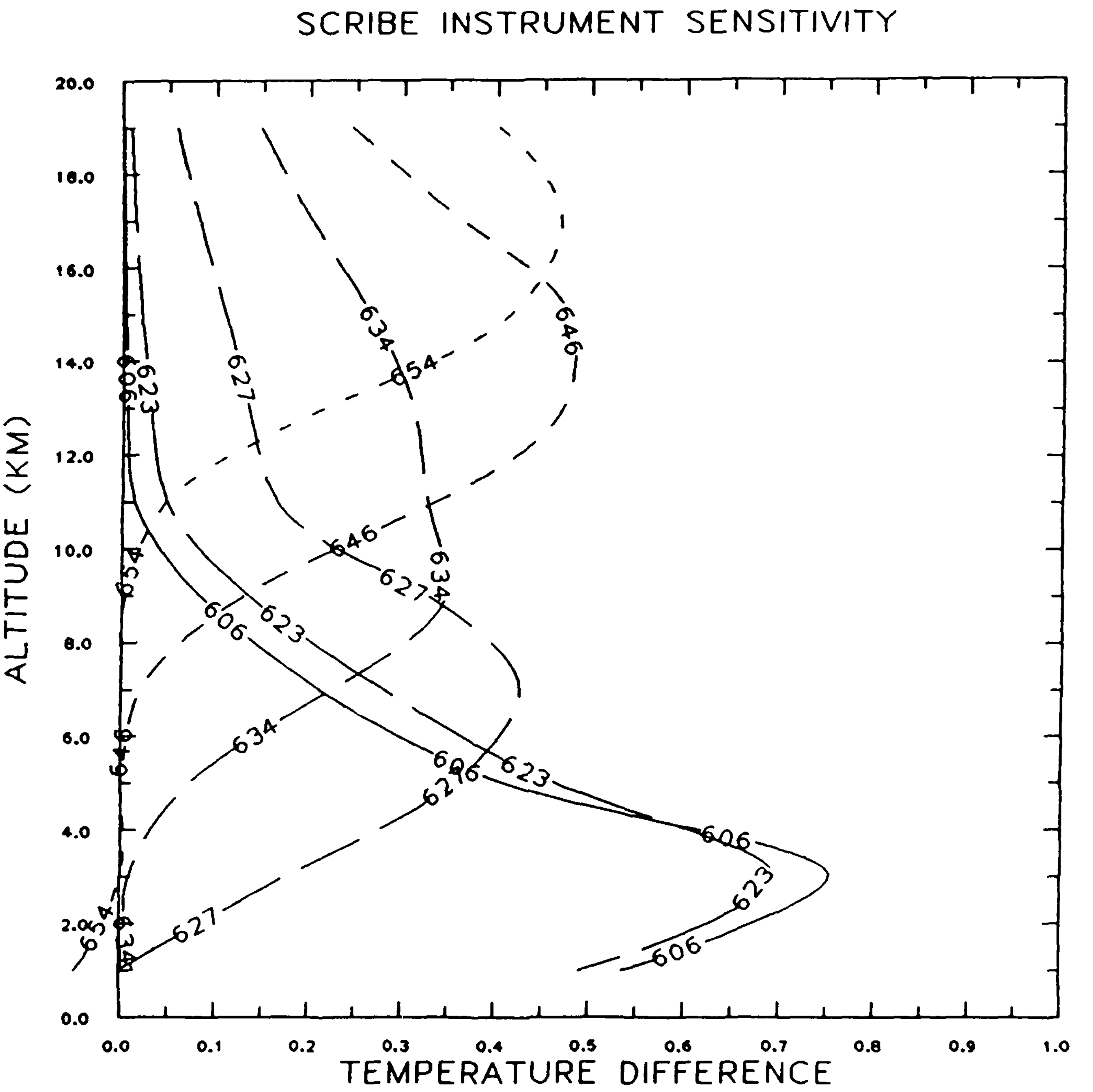


Figure 13 SCRIBE instrument sensitivity results: 606-669 cm^{-1} channels, old line data, US standard atmosphere, with line coupling calculated for 230K.

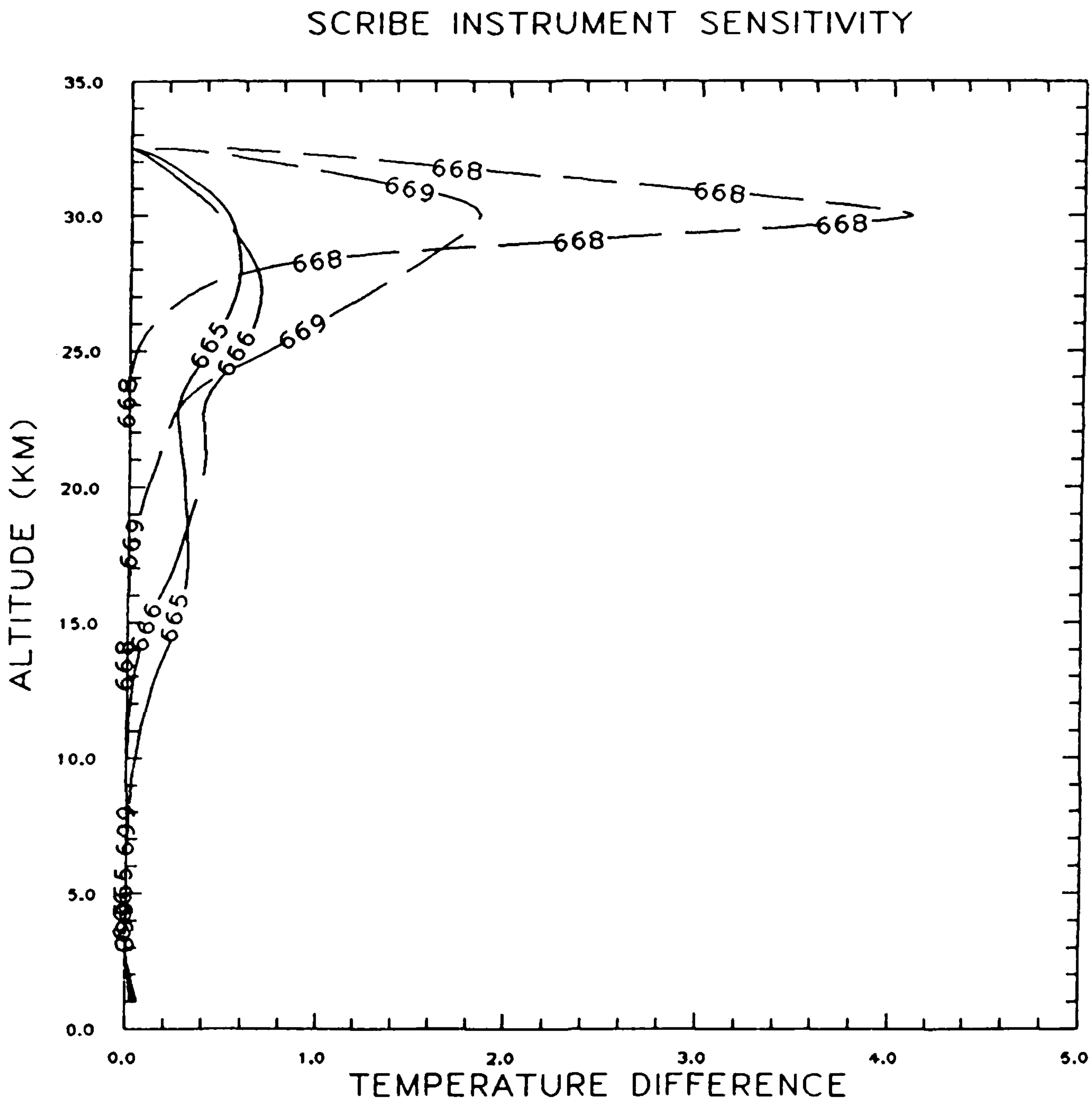


Figure 14 SCRIBE instrument sensitivity results: 665-669 cm^{-1} channels, new line data, US standard atmosphere, with line coupling calculated for 230K.

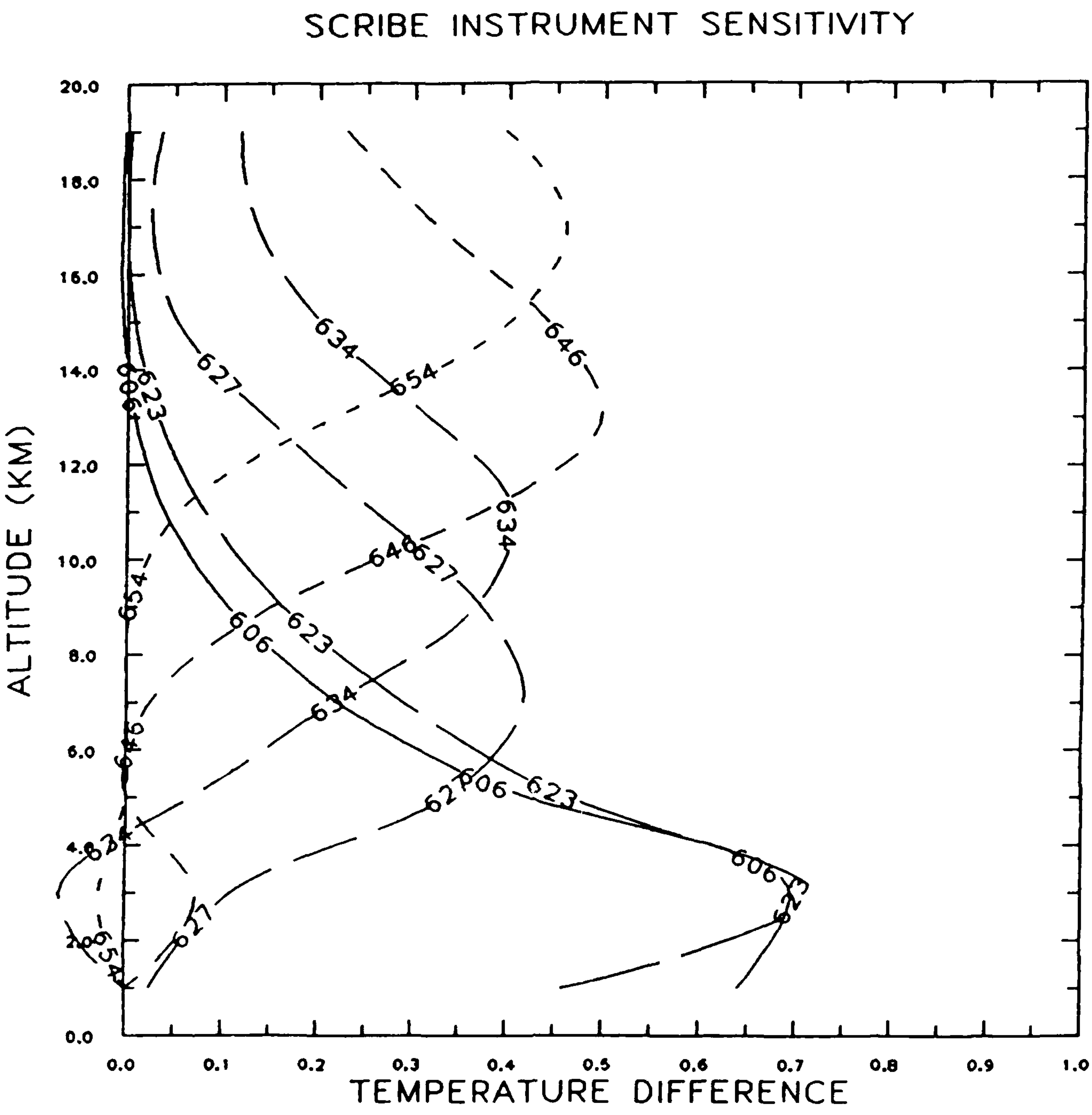


Figure 15 SCRIBE instrument sensitivity results: 606-654 cm^{-1} channels, new line data, tropical atmosphere, with line coupling calculated for 230K.

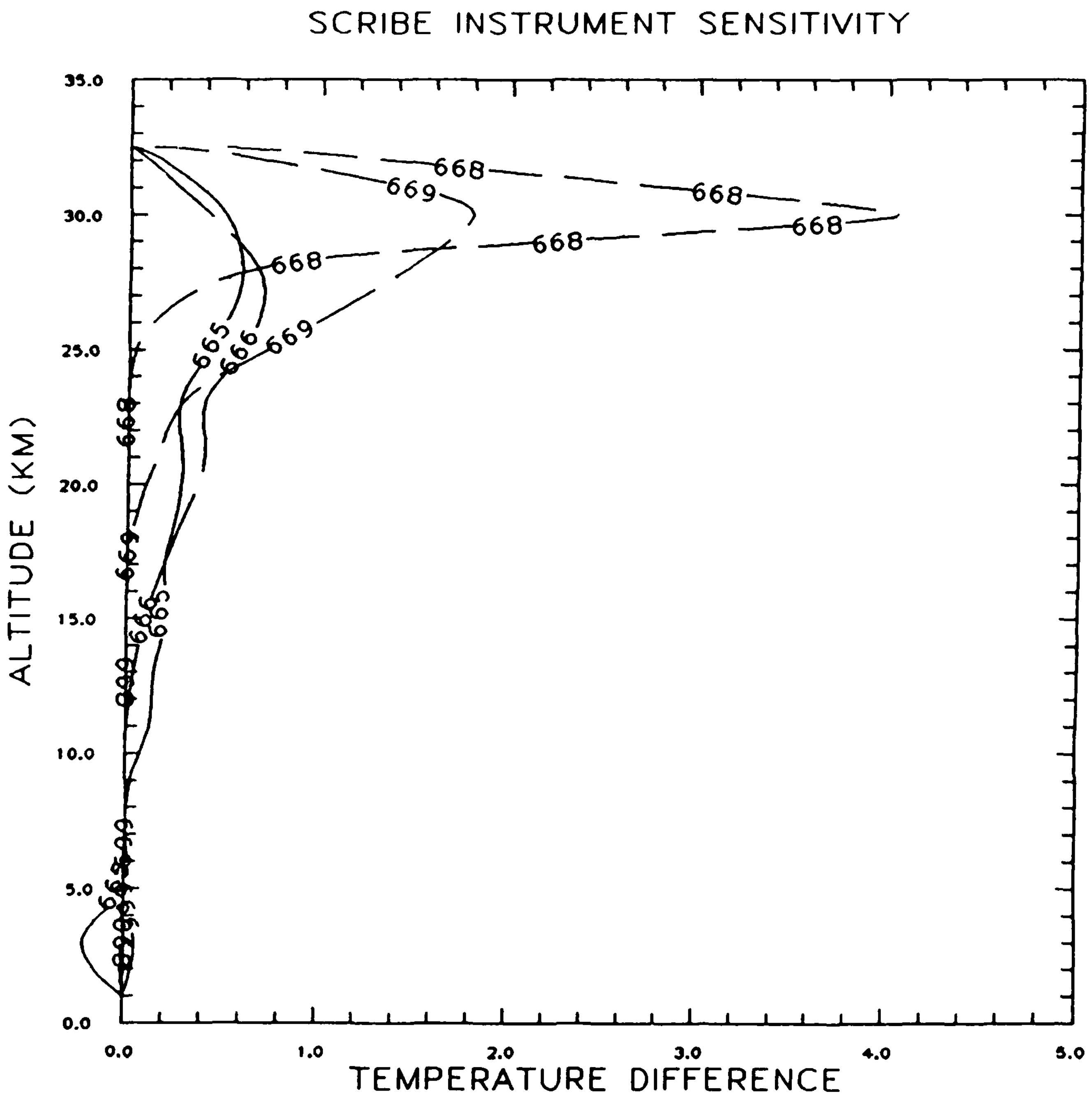


Figure 16 SCRIBE instrument sensitivity results: 665-669 cm^{-1} channels, new line data, tropical atmosphere, with line coupling calculated for 230K.

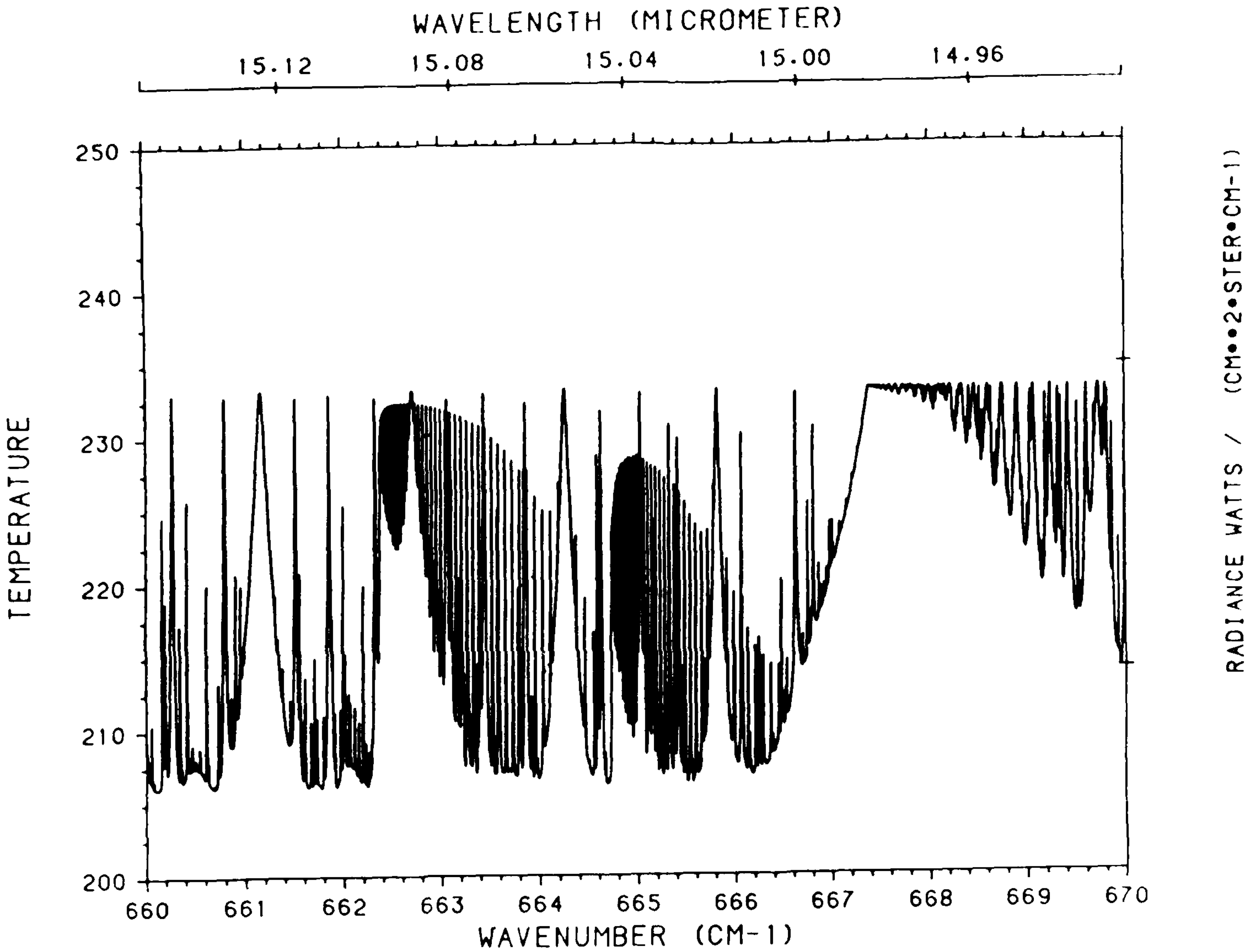


Figure 17 FASCODE simulation of SCRIBE nadir data for the 660-670 cm^{-1} range (no line coupling). (in deg K)

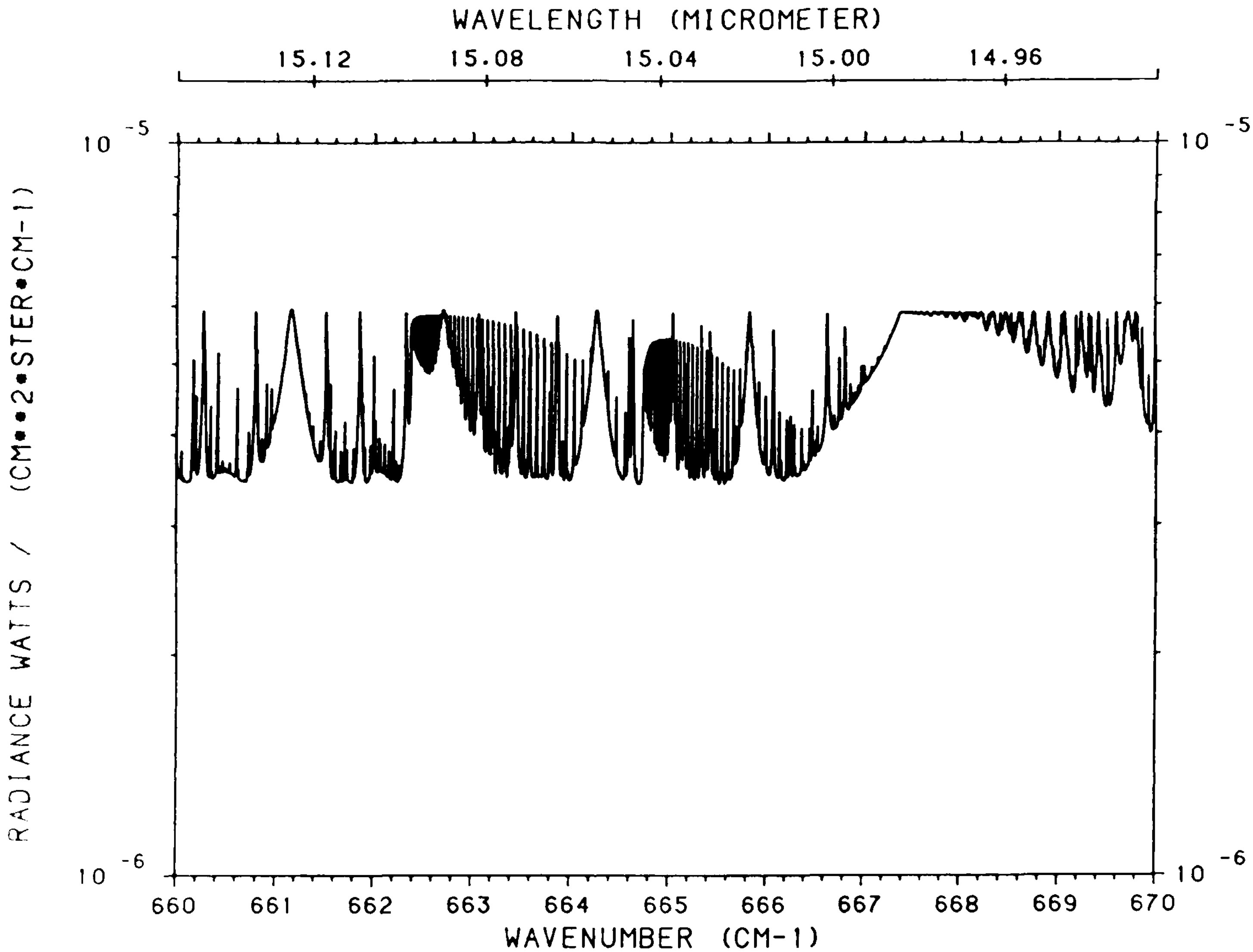


Figure 18 FASCODE simulation of SCRIBE nadir data for the 660-670 cm^{-1} range (no line coupling). (radiance)

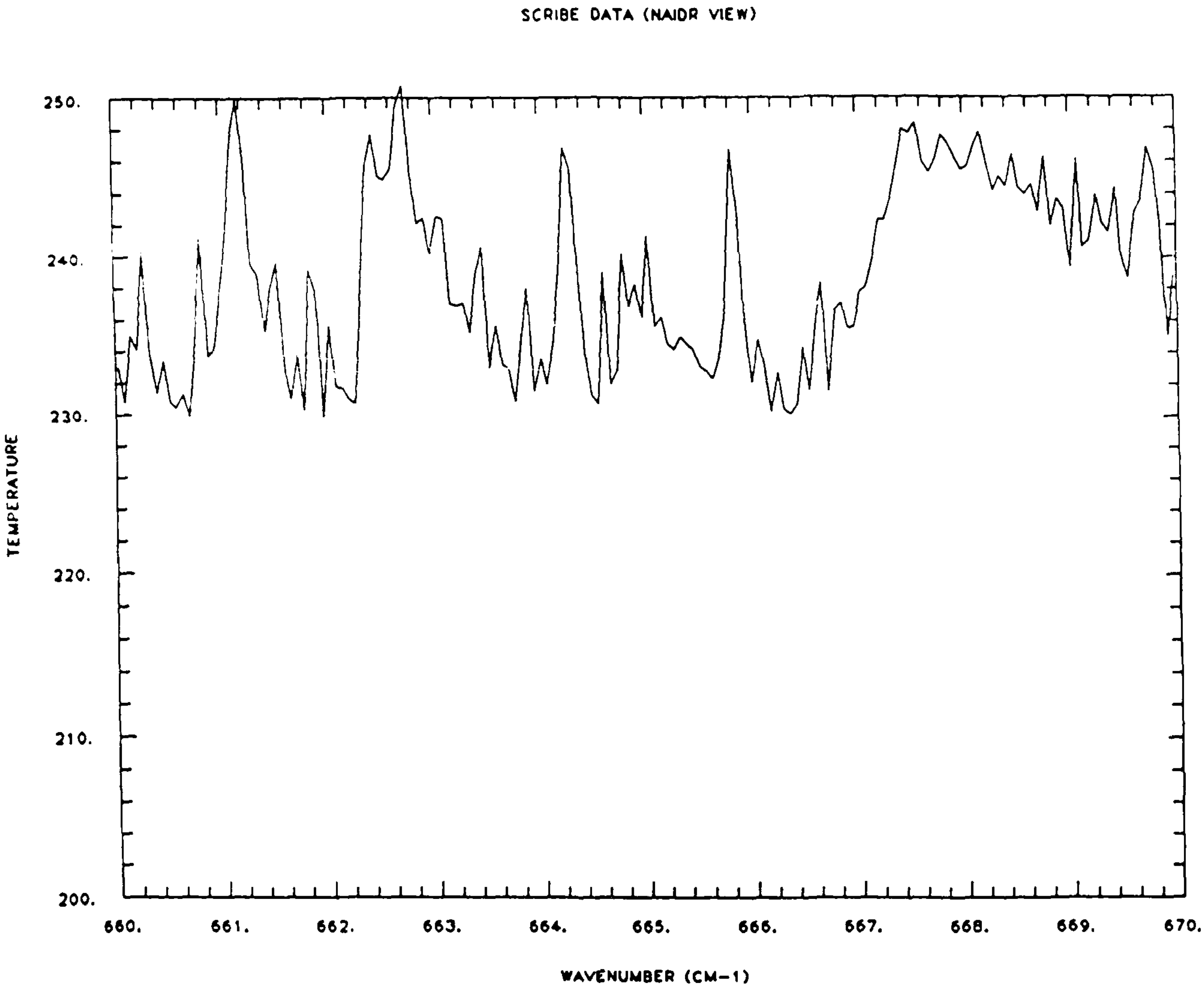


Figure 19 SCRIBE data, nadir view, 660-670 cm^{-1}. (in deg K)

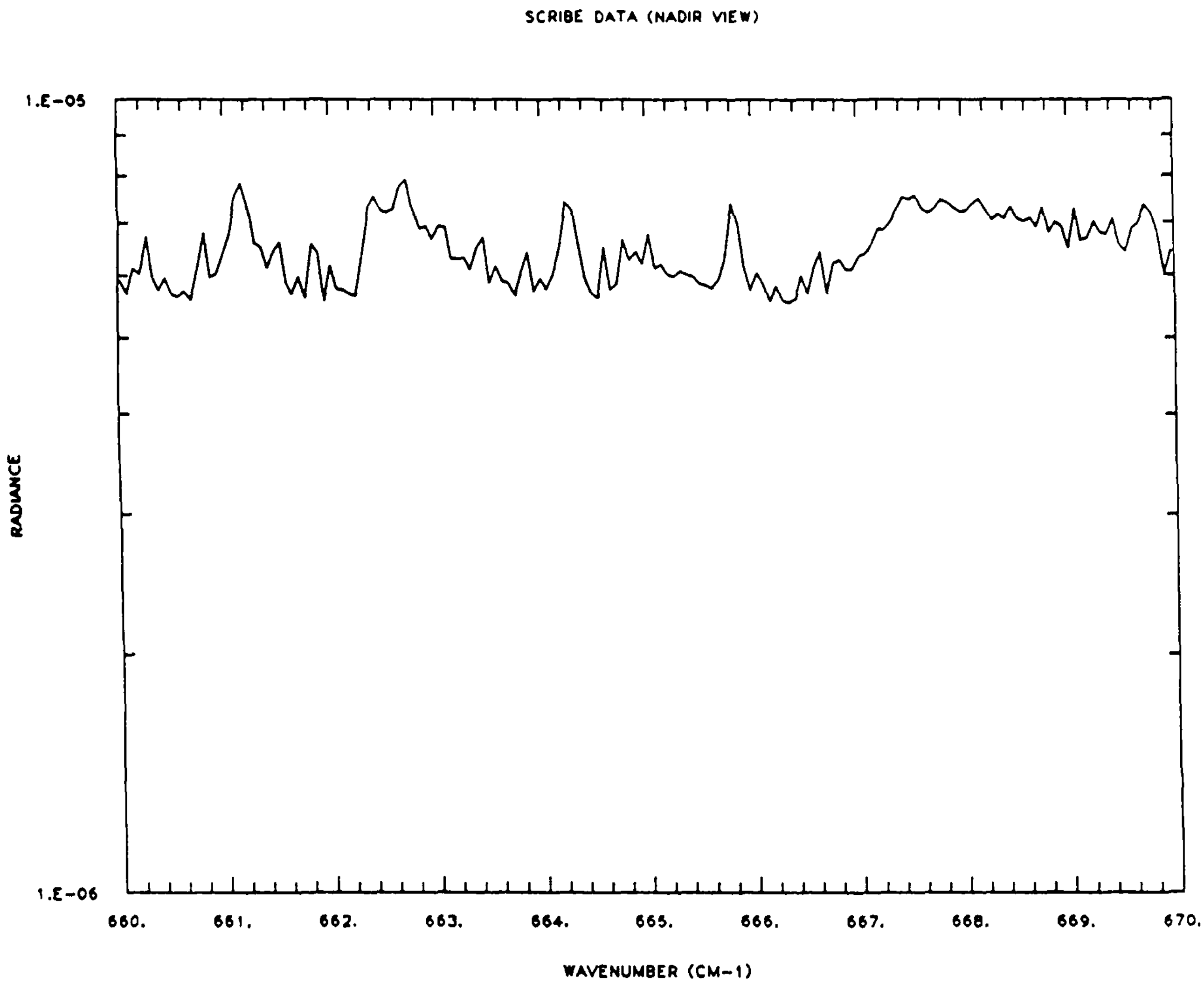


Figure 20 SCRIBE data, nadir view, 660-670 cm^{-1}. (radiance)

To investigate potential effects of line coupling on the spectra in the immediate vicinity of the Q branch, synthetic spectra were evaluated with and without line coupling effects in the reduced wavenumber domain from 666.5 to 668.0 cm^{-1}. This spectrum (without line coupling) is illustrated in Figure 21. Figure 22 shows the same result, however including line coupling effects based on Hoke's coupling coefficients for 210K. The reduced wavenumber domain was chosen to isolate a spectral region whose emission could be characterized by assuming a quasi-isothermal layer at 210K to facilitate the line coupling calculation The simulations with and without line coupling (Figures 22 and 21, respectively) can be compared to the observed SCRIBE spectrum (Figure 23). The reduced radiance from 666.5 to 667.3 cm^{-1} can be attributed to a decreased absorption coefficient induced by line coupling in the part of the stratosphere below the SCRIBE level where the temperature increases with height, i.e., SCRIBE "sees" less warm and more cold air because of line coupling. These results help explain the effects of line coupling on the sensitivity curves. The 666.8 cm^{-1} channel is centrally located in the spectral region where there is maximum weakening of the absorption coefficient from line coupling and therefore should show, as it does, greatest decrease in sensitivity. The channels at 668.2 and 669.4 cm^{-1} are so opaque that even a large relative change in absorption coefficient should not affect the opacity.

Figures 24 to 25 present detailed synthetic spectra as in Figures 17 and 18, but for limb viewing at a zenith angle of 93.7°. The corresponding measured SCRIBE spectra, shown in Figures 26 and 27, do not seem to have the residual calibration problems that the nadir spectra do. Again, the calculated line coupling effects are evidenced by a reduced radiance. This can be seen by comparing Figure 28 and 29 (no line coupling and line coupling, respectively). The agreement between the observed spectrum (Figure 30) and the calculation is improved by the incorporation of the line coupling effect. In this case, that is to be expected because the viewing tangent height is about 17 km, so that most of the trajectory is through an atmospheric path at heights where the temperature is less than 210K. In the opaque spectral regions, where the brightness temperatures are higher, the tangent height temperature is irrelevant, as are line coupling effects.

For limb scanning, the agreement between calculated and measured spectra is at least as good as for nadir viewing. Again the effects are potentially very important, and again the temperature dependence of these effects are even more so.

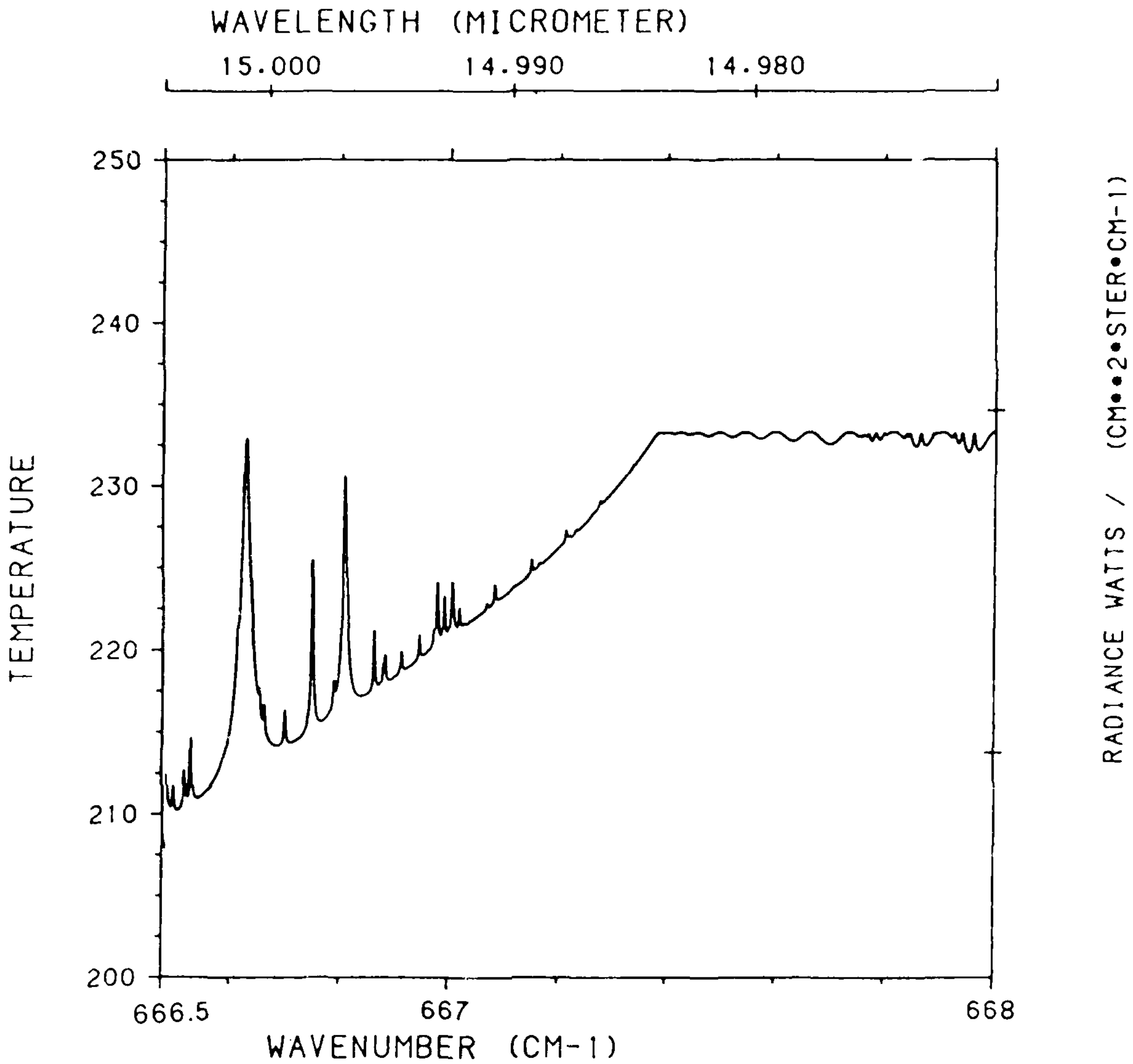


Figure 21 FASCODE simulation of SCRIBE nadir data for the 666.5-668 cm^{-1} range (no line coupling). (in deg K)

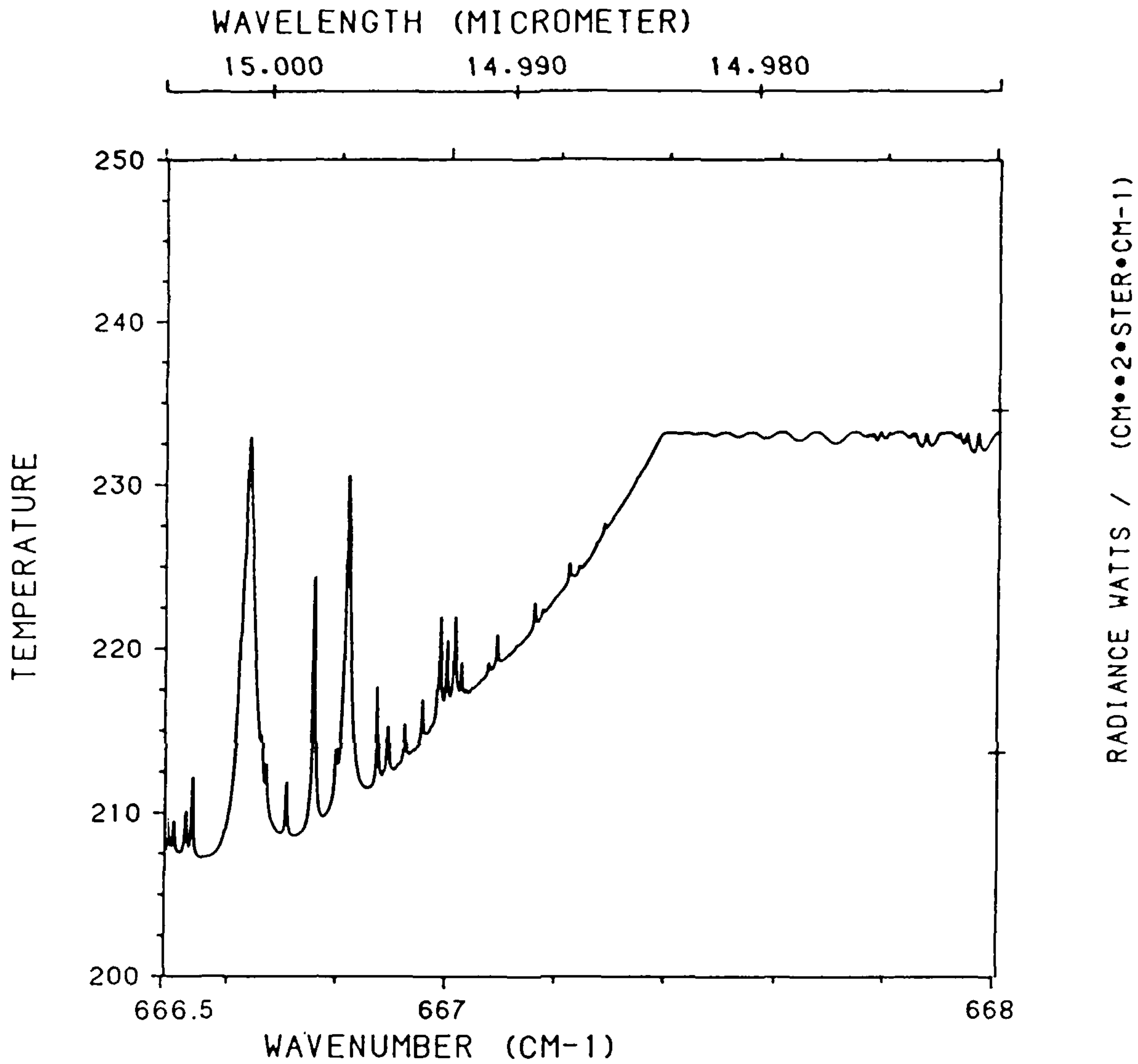


Figure 22 FASCODE simulation SCRIBE nadir data including line coupling calculated for 210K for 666.5-668 cm^{-1} range. (in deg K)

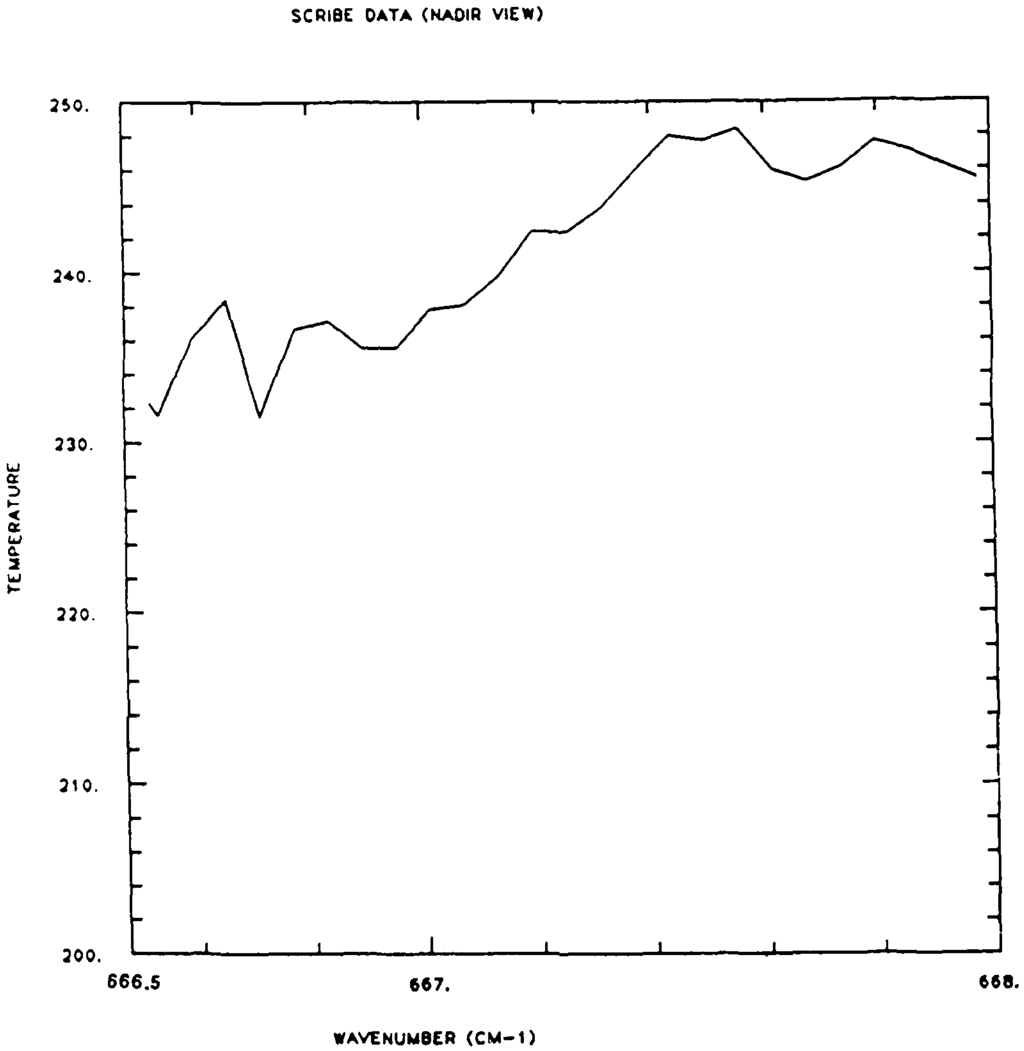


Figure 23 SCRIBE data, nadir view, 666.5-668 cm^{-1}. (in deg K)

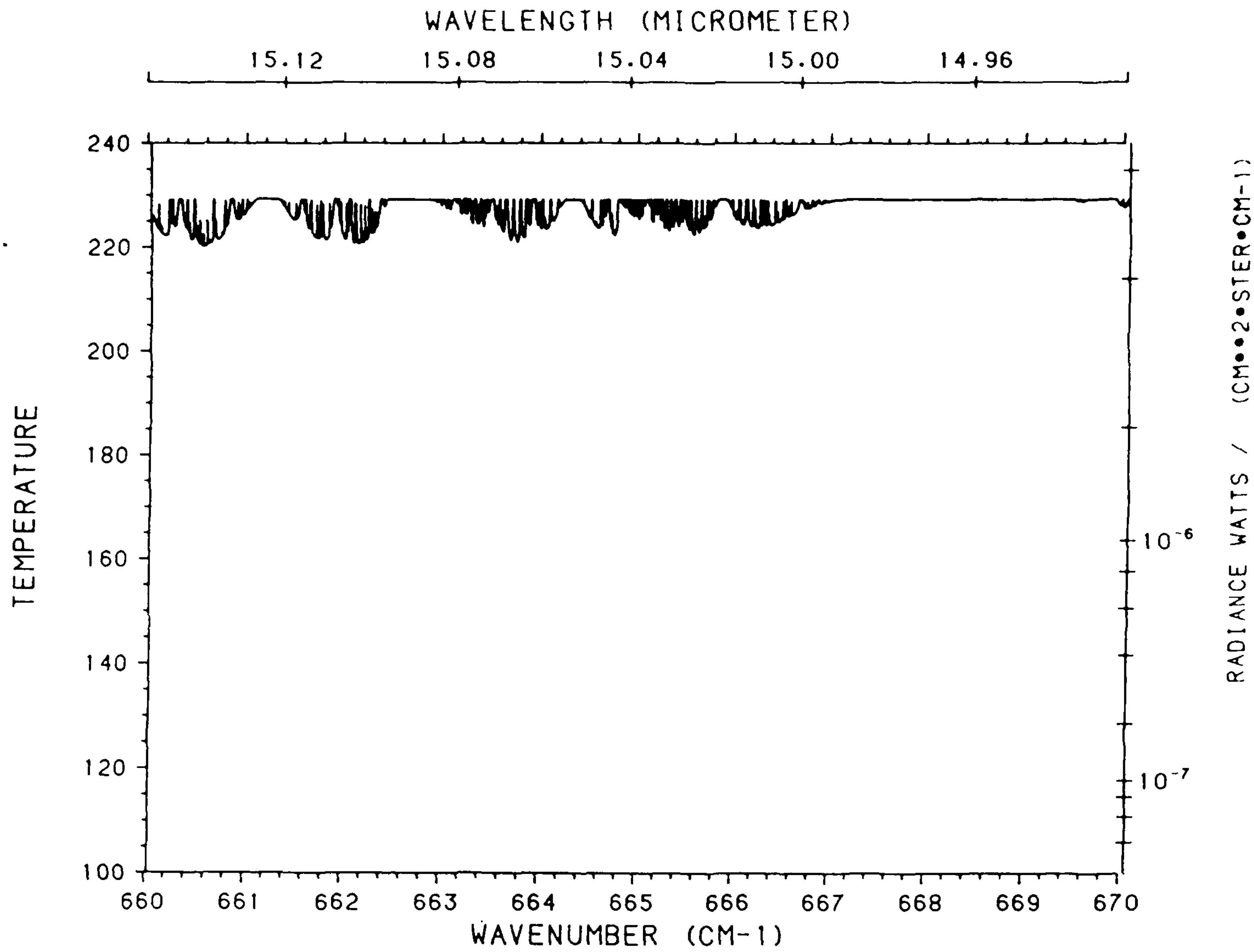


Figure 24 FASCODE simulation of SCRIBE limb data for the 660-670 cm^{-1} range (no line coupling). (in deg K)

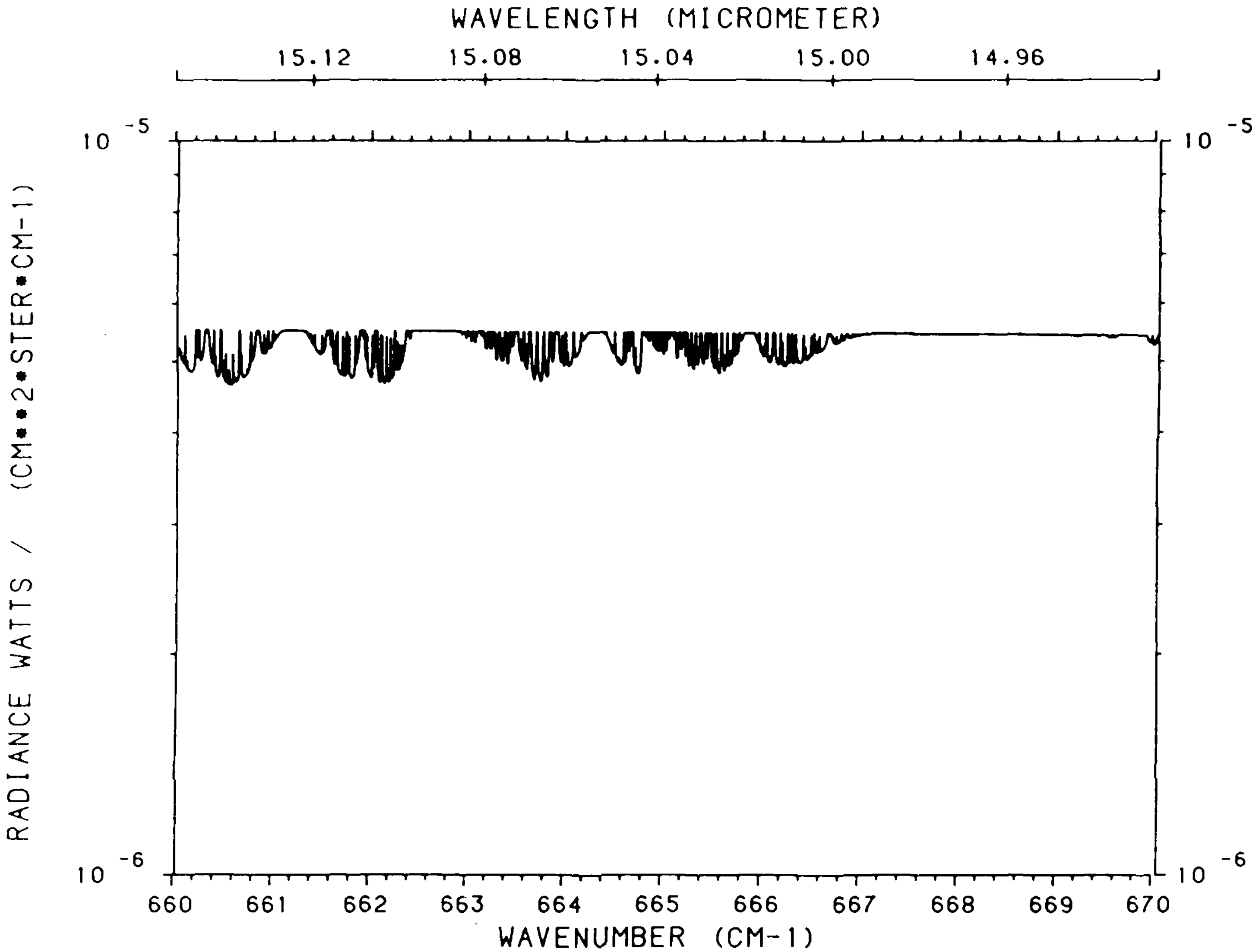


Figure 25 FASCODE simulation of SCRIBE limb data for the 660-670 cm^{-1} range no line coupling). (radiance)

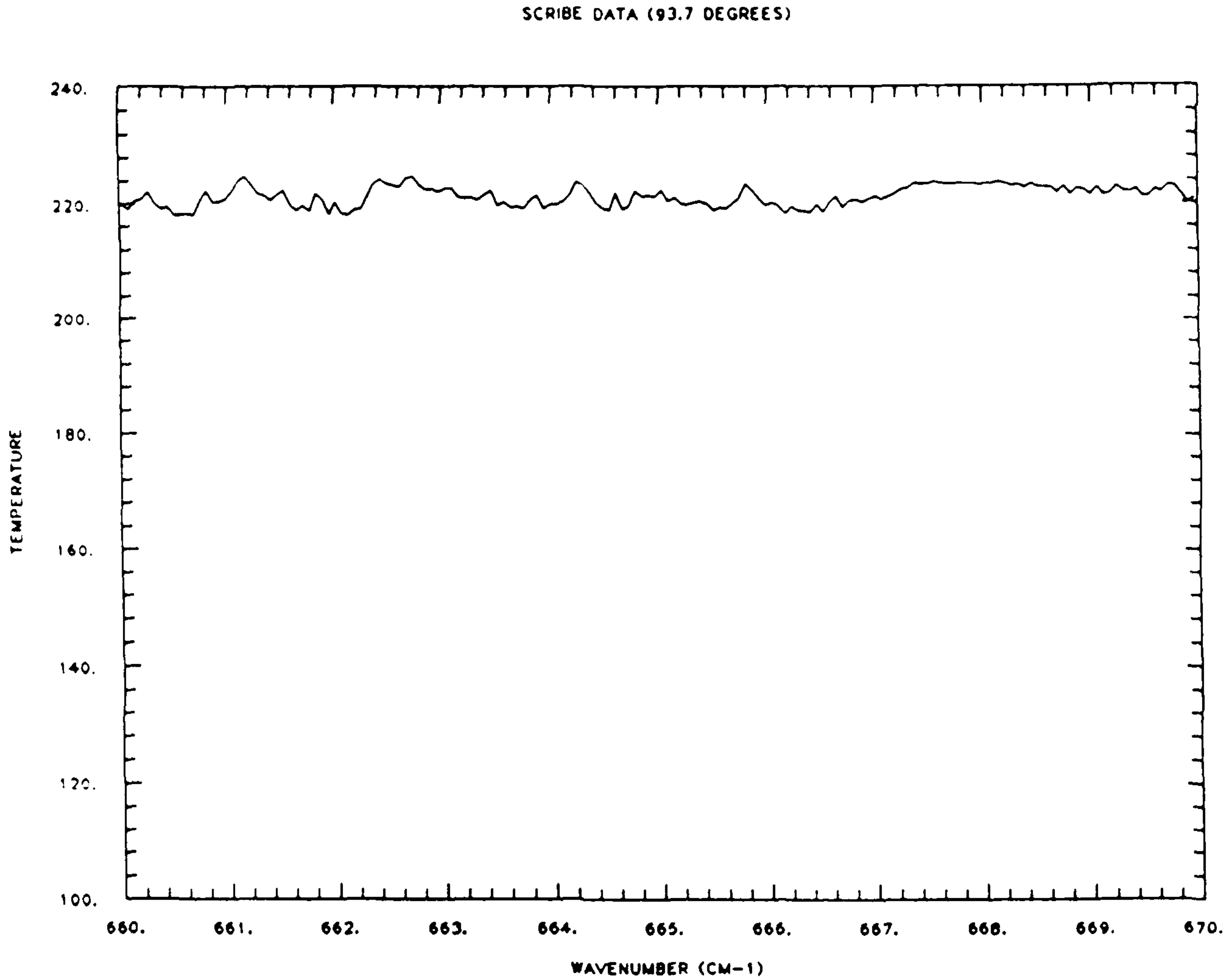


Figure 26 SCRIBE data, limb view, 660-670 cm^{-1}. (in deg K)

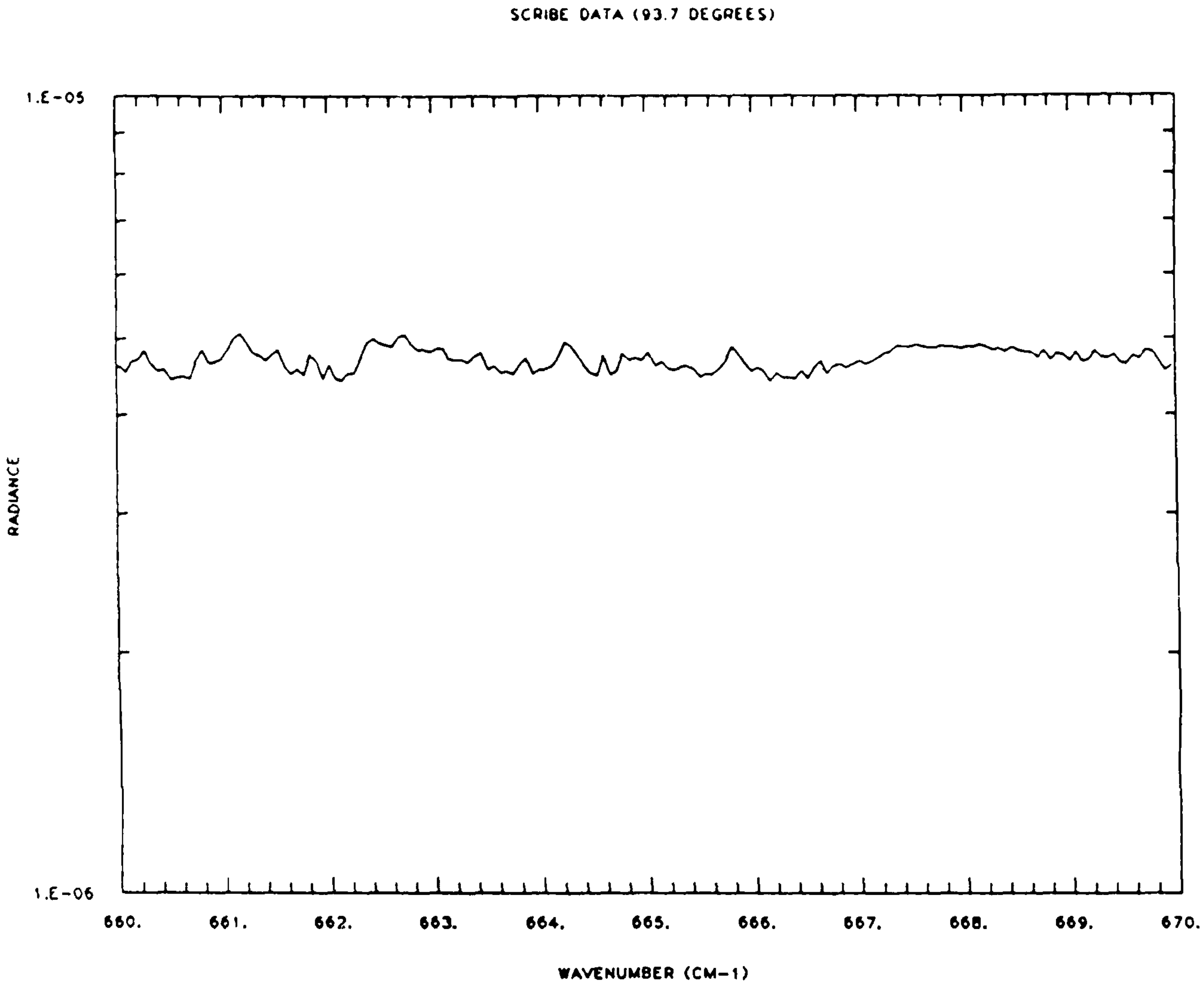


Figure 27 SCRIBE data, limb view, 660-670 cm^{-1}. (radiance)

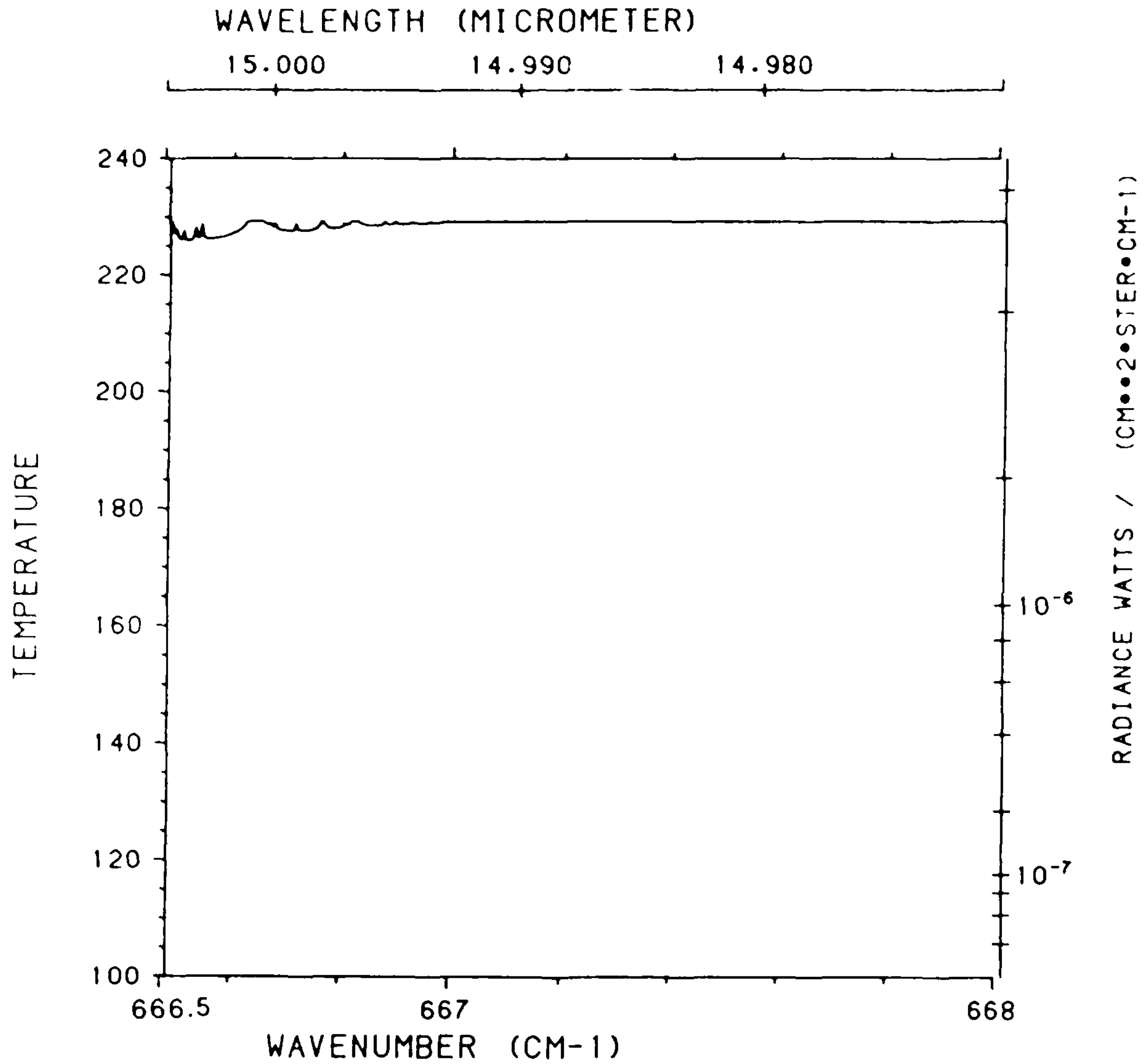


Figure 28 FASCODE simulation of SCRIBE limb data for the 666.5-668 cm^{-1} range (no line coupling). (in deg K)

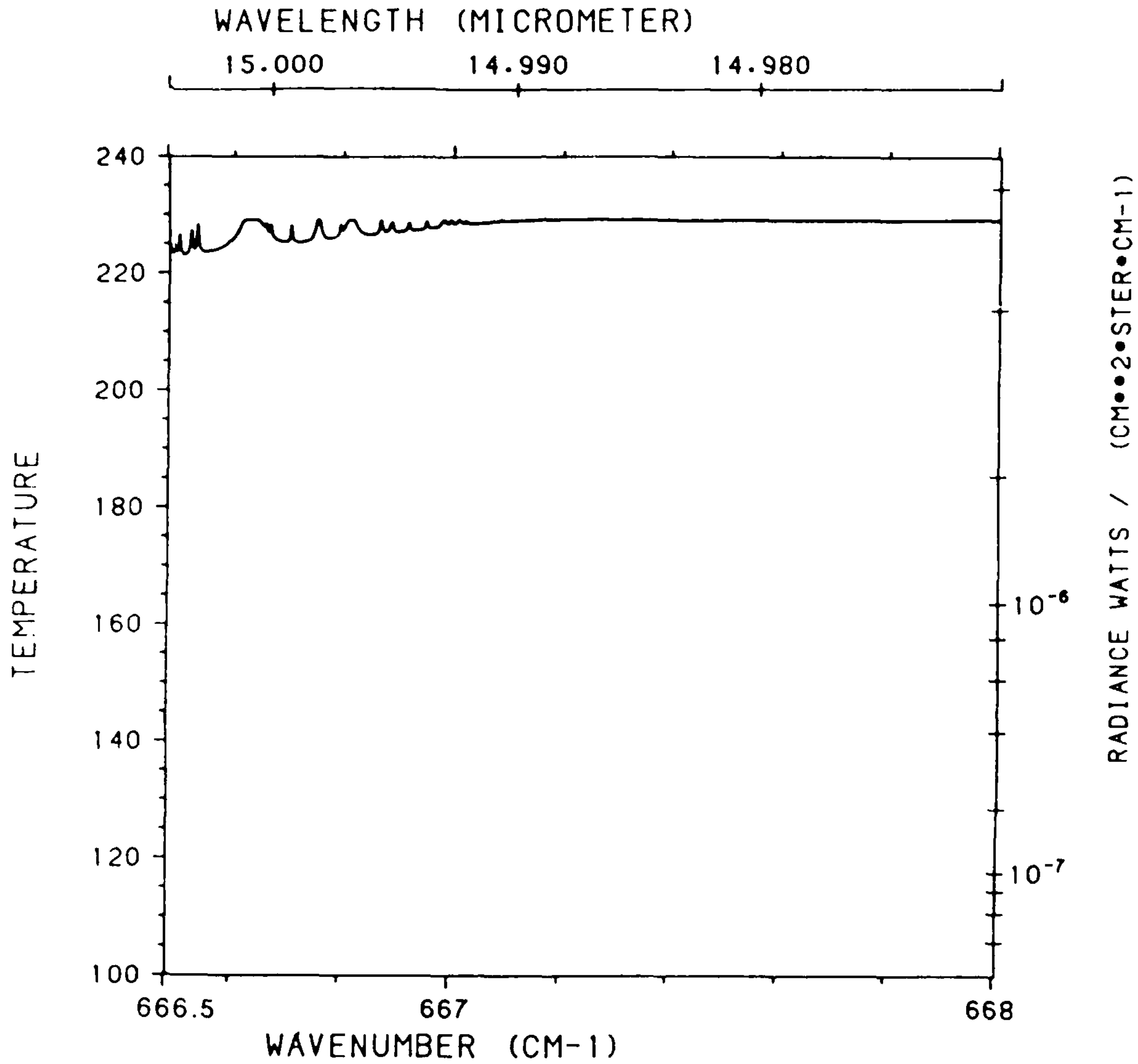


Figure 29 FASCODE simulation of SCRIBE limb data including line coupling calculated for 210K for 660-670 cm^{-1} range. (in deg K)

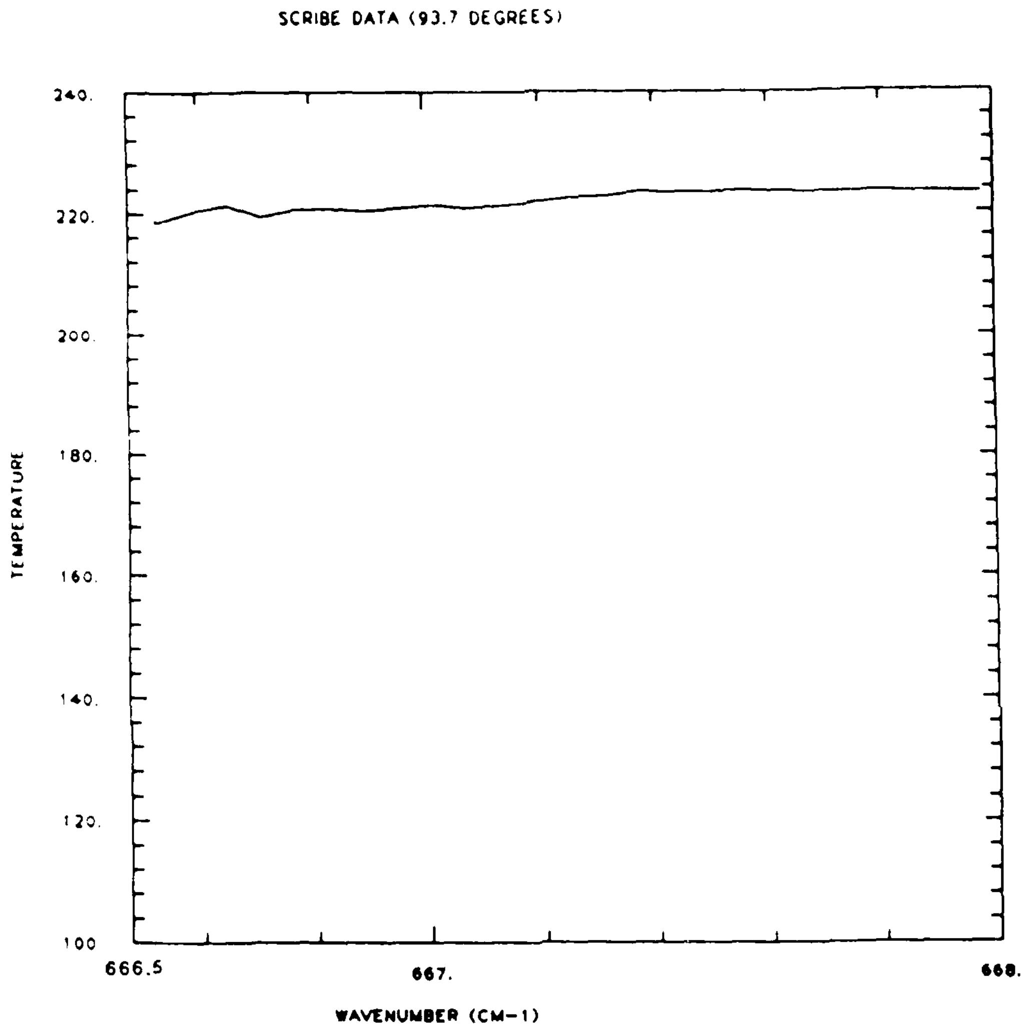


Figure 30 SCRIBE data, limb view, 666.5-668 cm^{-1} (in deg K)

5. Conclusions and Recommendations

5.1 Summary

We have developed a FASCODE routine for calculating synthetic radiances that would be received at SCRIBE level and viewing angle, and used this routine to conduct temperature retrieval studies and to investigate the effect of line coupling on radiances.

Physical retrievals obtained with the use of the AMTS 15 μm channels were found to be sensitive to the first guess to the solution. A series of sensitivity studies were carried out and resulted in finding a nicely spaced universal set of heights to which the tropospheric channels could correspond in relaxation-type retrievals. Well-resolved stratospheric temperature retrievals probably require limb scanning.

Line coupling was found to have strong effects on atmospheric radiances and to be temperature sensitive. It seems to have the potential for being particularly important in the troposphere, and may be useful for remote location of the tropopause.

The SCRIBE spectra are ideal for these types of study.

5.2 Recommendations

It is strongly recommended that study and interpretation of the SCRIBE data be continued and expanded, with emphasis on both retrieval studies and line coupling effects.

More work should be done on calibrating the spectra, and the new 1986 spectra should be calibrated, studied and used. It is clear from our comparison between synthetic and actual spectra that there are discrepancies which require further investigation. More SCRIBE spectra should be taken, and extended to other spectral regions. There is much to be obtained from them.

The retrieval studies undertaken in this initial phase of our research provide the baseline capabilities for exploiting the extensive information content of the SCRIBE spectra. The sensitivity calculations have provided the background for selection of an optimal channel set for temperature retrieval studies. Limited resources in the initial effort preclude taking advantage of the temperature retrieval capability at this time. Similar considerations apply to the development of analogous constituent retrieval capabilities for which the temperature retrieval is a necessary prerequisite. Approaches have been developed for constituent channel selection and related sensitivity studies.

To significantly improve retrieval efficiency, rapid algorithm retrieval routines should be developed for the specified SCRIBE sounding channels. To enhance the applicability of the FASCOD2 forward problem calculation, variable temperature dependence of the line coupling coefficients should be incorporated in the FASCODE program and also in the rapid algorithm routines, if possible, and programs should be developed for obtaining temperature and constituent retrievals from limb sounding.

Examination of line coupling effects should be extended to other CO_2 Q-branches in the 15 μm complex and to Q-brances of freons, C NO_3, O_3, etc. The effect of line coupling on remote sensing of temperatue and constituent concentrations should be investigated further taking advantage of the FASCOD2-based retrieval capability developed here and its future enhancements.

6. Acknowledgements

The authors thank Dr. Michael Hoke of AFGL for kindly providing calculations of temperature dependent line coupling coefficients in support of our work and Bill Gallery of OPtiMetrics for supplying SCRIBE spectra and information on their reliability and accuracy. Dr. Aaron Goldman of the University of Denver provided details on instrument calibration and idiosyncracies and spectra to be compared with the OPtiMetrics data base. James Chetwynd of AFGL was helpful in circumventing the various potential pitfalls in the use of FASCOD2.

We also gratefully acknowledge the support and encouragement of George Vanasse and Dr. Laurence Rothman of AFGL in this work.

This report was competently word processed by T. Foley and B. Bruso of AER.

7. References

Chahine, M. T., N. L. Evans, V. Gilbert, and R. D. Haskins, 1984: Requirements for a passive IR advanced moisture and temperature sounder. Appl. Opt., 23, 7, 979-989.

Clough, S. A., F. X. Kneizys, E. P. Shettle, and G. P. Anderson, 1986: Atmospheric Radiance and Transmittance: FASCOD2. Proceedings, Sixth Conference on Atmospheric Radiation. American Meteorological Society. pp. 141-144.

Isaacs, R. G., R. N. Hoffman, and L. D. Kaplan, 1986a: Remote sensing of geophysical parameters for numerical weather prediction. Reviews of Geophys.,24, 4, 701-743.

Murcray, F. H., F. J. Murcray, D. G. Murcray, J. Pritchard, G. Vanasse, and H. Sakai, 1984: Liquid nitrogen-cooled Fourier transform spectrometer system for measuring atmospheric emission at high altitudes. J. Atmos. Ocean. Technology, 1, 351-357.

Murcray, D. G., F. H. Murcray, F. J. Murcray, and G. Vanasse, 1985: Measurements of atmospheric emission at high spectral resolution. J. Meteorl. Soc. Japan, 63, 320-324.

Rothman, L. S., R. R. Gamache, A. Barbe, A. Goldman, J. R. Gillis, L. R. Brown, R. A. Toth, J.-M. Flaud, and C. Camy-Peyret, 1983: AFGL atmospheric line parameters compilation. Appl. Opt., 22, 2247-2256.

Susskind, J., J. Rosenfield, D. Reuter and M.T. Chahine, 1982: private communication

END

10-87

DTIC